

# **USING ADVANCED COMPUTING IN APPLIED DYNAMICS: FROM THE DYNAMICS OF GRANULAR MATERIAL TO THE MOTION OF THE MARS ROVER**

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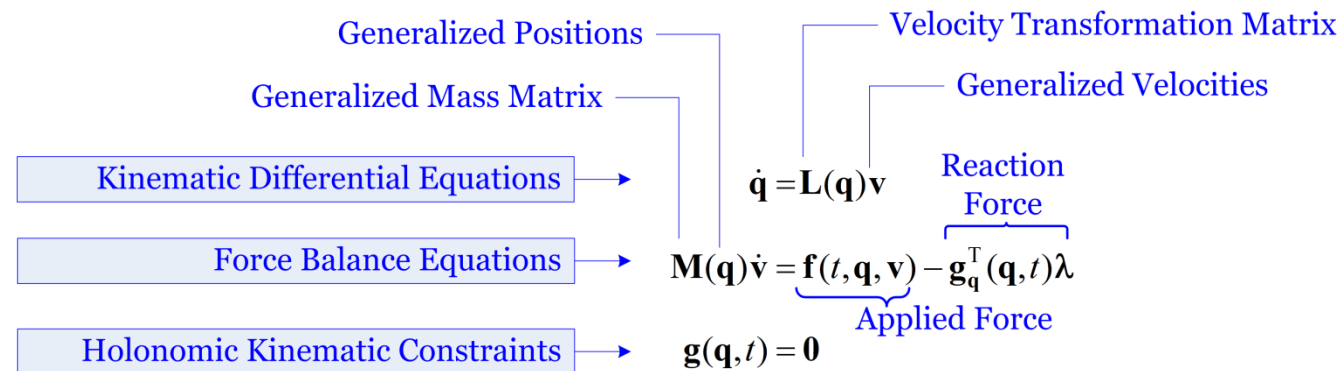
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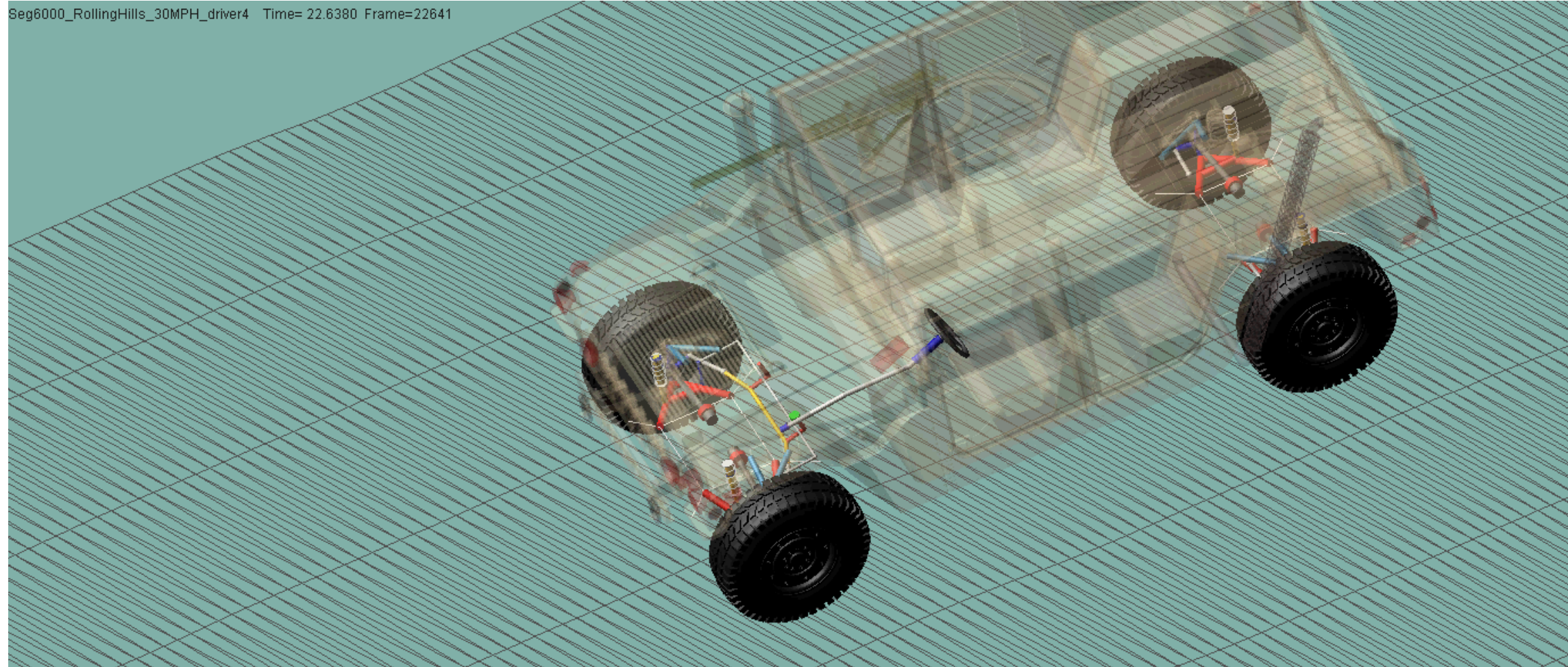
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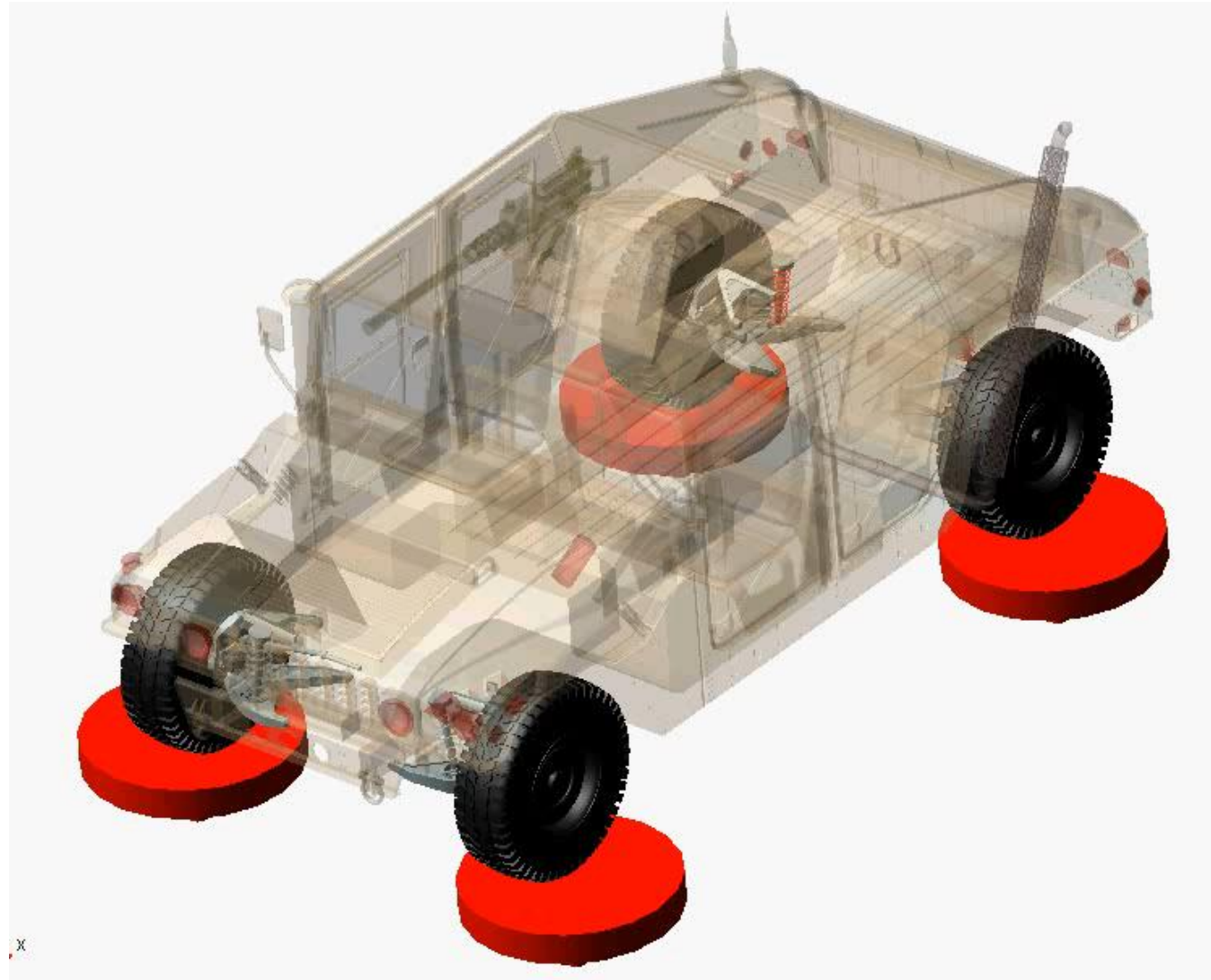
# Classical Computational Multibody Dynamics: Newton-Euler Constrained Equations of Motion



# Multibody Dynamics: What is it? [commercial software simulation]



# Multibody Dynamics: What is it? [commercial software simulation]





## Example Open Problem: Mobility on Deformable Terrain

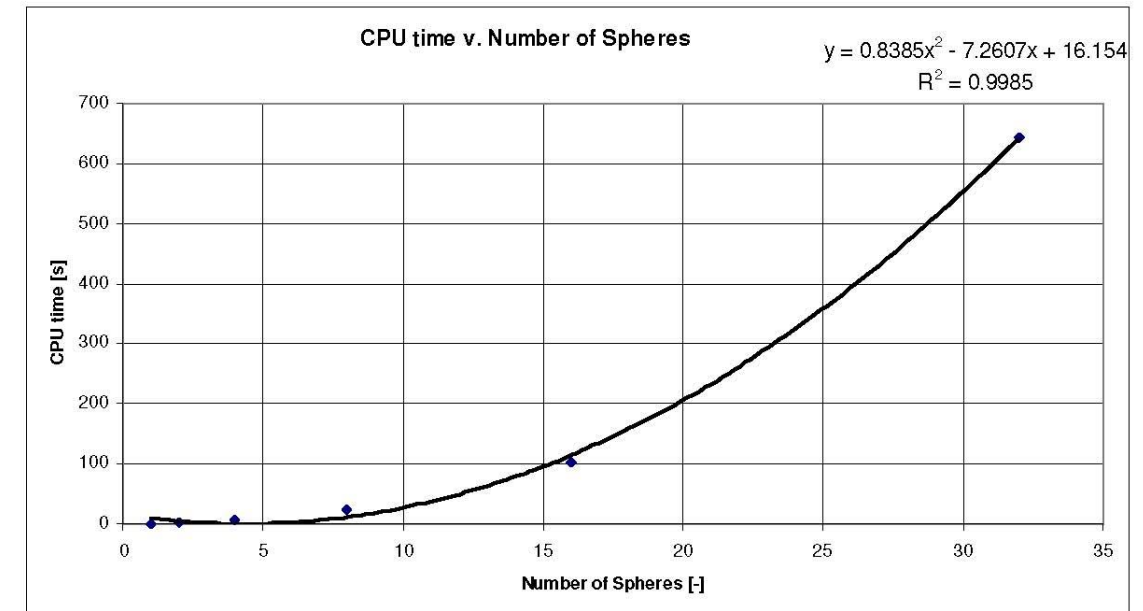
- How is the Rover moving along on a slope with granular material?
- What wheel geometry is more effective?
- How much power is needed to move it?
- At what grade will it get stuck?
- And so on...



# Frictional Contact Simulation

## [Commercial Software Simulation - 2007]

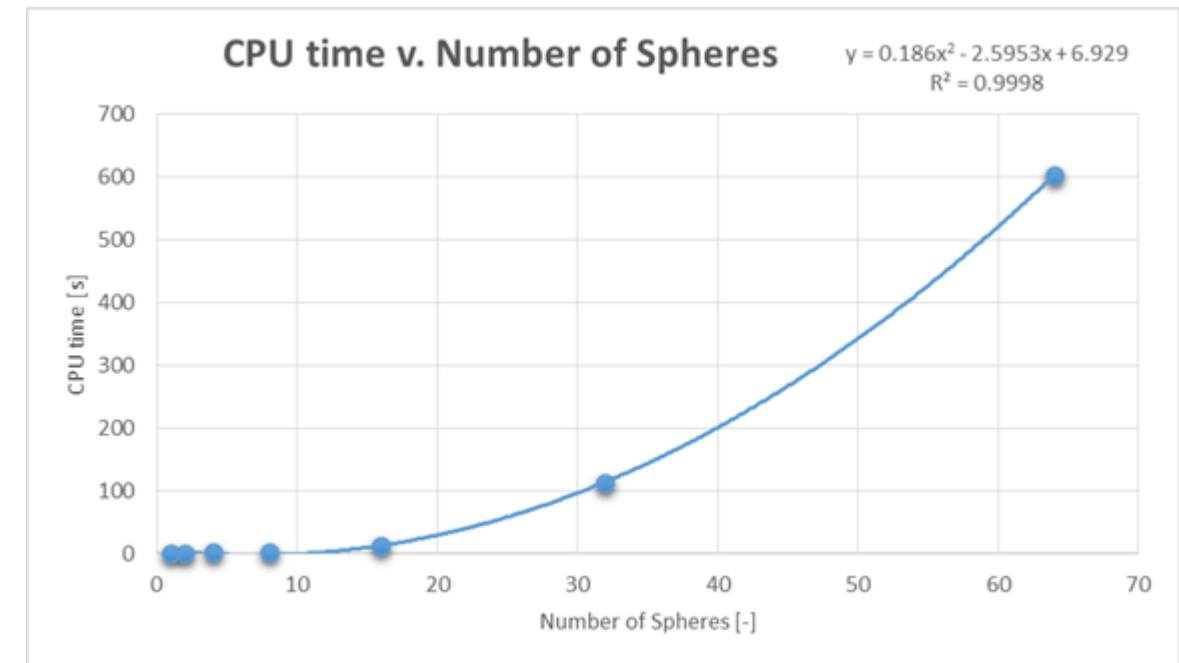
- Model Parameters:
  - Spheres: 60 mm diameter and mass 0.882 kg
  - Penalty Approach: stiffness of  $1E5$ , force exponent of 2.2, damping coefficient of 10.0
  - Simulation length: 3 seconds



# Frictional Contact Simulation

## [Commercial Software Simulation - 2013]

- Same problem tested in 2013
- Simulation time reduced by a factor of six
- Simulation times still prohibitively long

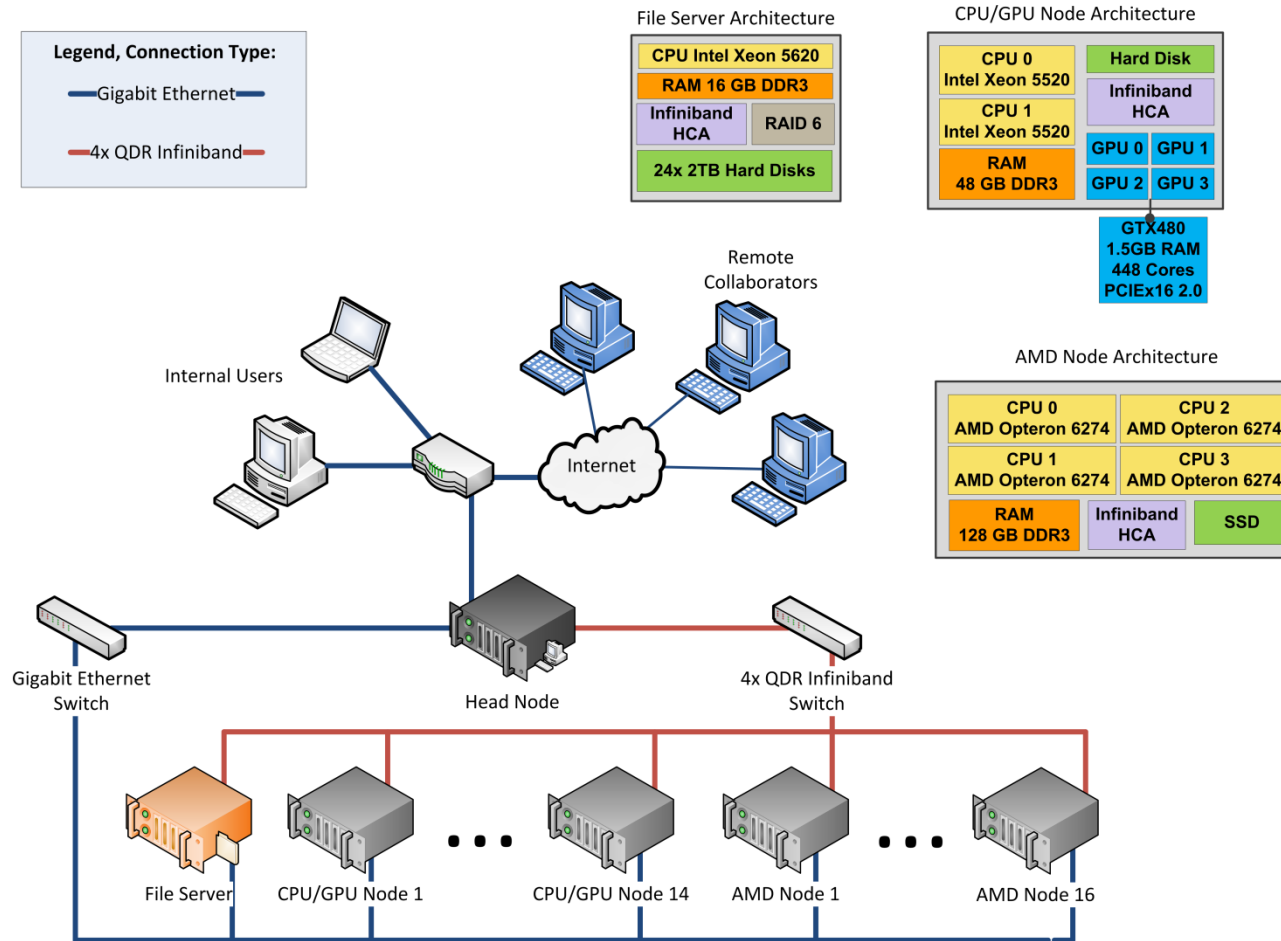


# Why It's Worth Reconsidering Challenging Problems...





# Lab's Research Heterogeneous Cluster



# Lab's Research Heterogeneous Cluster

- More than 50,000 GPU scalar processors
- More than 1,200 CPU cores
- Fast Mellanox Infiniband Interconnect (QDR), 40Gb/sec
- About 2.7 TB of RAM
- More than 20 Tflops Double Precision

The issues is not hardware availability. Rather, it is producing modeling and solution techniques that can leverage the hardware

# CHRONO:

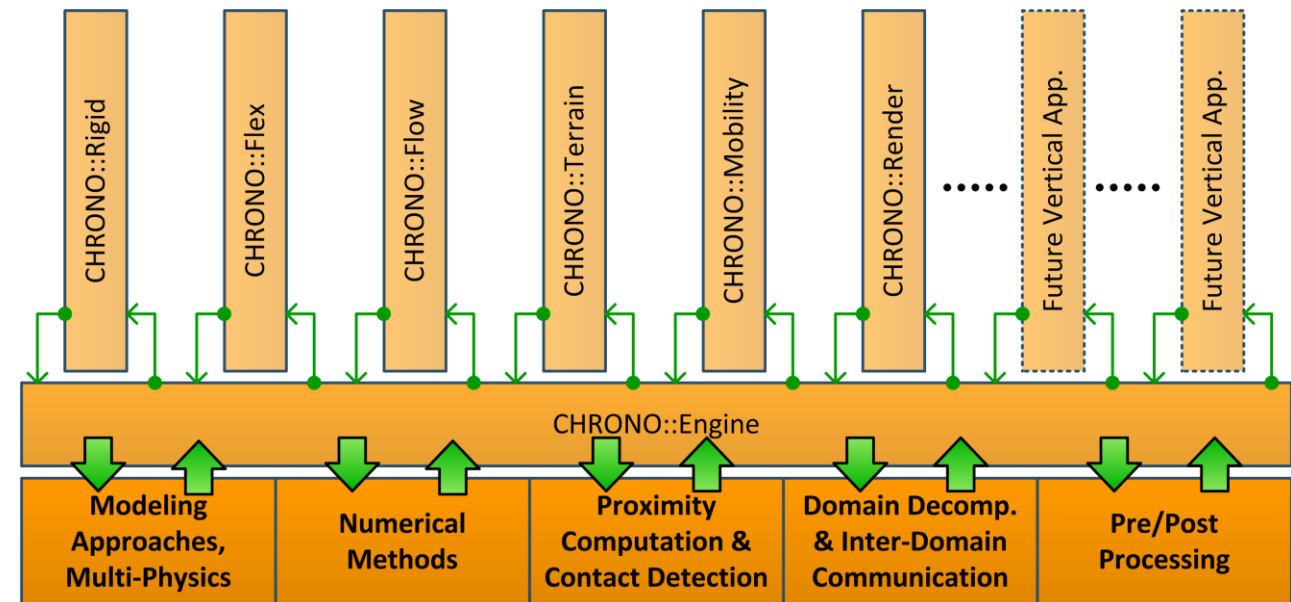
## Research-Grade Software Infrastructure for Multi-physics Modeling/Simulation/Visualization

- Goal: advance state of the art in modeling, simulation, and visualization
  - Use **emerging hardware** and novel algorithms to solve **open engineering problems**
  
- “**emerging hardware**” :
  - GPUs and clusters of CPUs
  
- “**open engineering problems**” :
  - Fluid-solid interaction, vehicle mobility, soil modeling, tire/terrain modeling, granular dynamics, etc.

# Chrono:

## Five Foundation Components

- Advanced modeling
- Solution methods
- Proximity computation
- Domain decomposition & Inter-domain data exchange
- Pre/Post-processing (visualization)



- **Chrono:**
  - Five foundation components support vertical apps

# Advanced Modeling Techniques

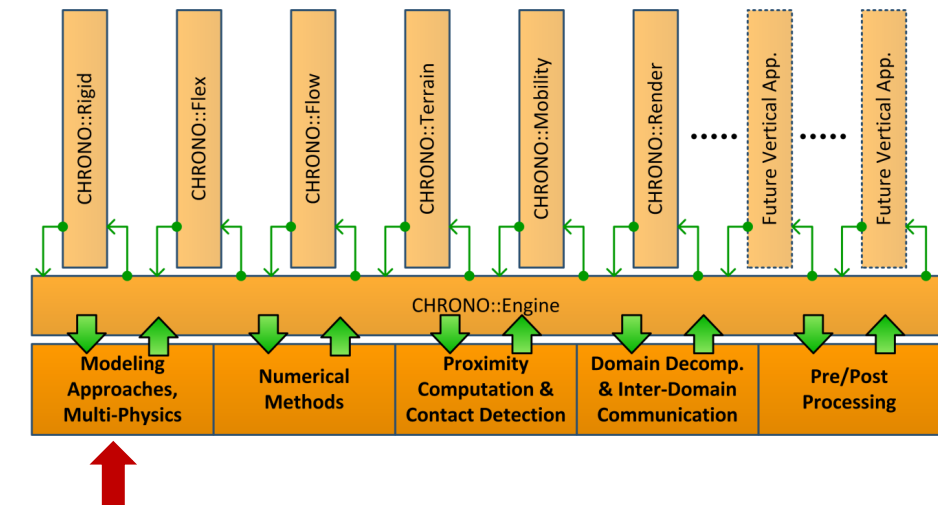
Advanced modeling techniques

Algorithmic (applied math) support

Proximity computation

Domain decomposition & Inter-domain data exchange

Post-processing (visualization)

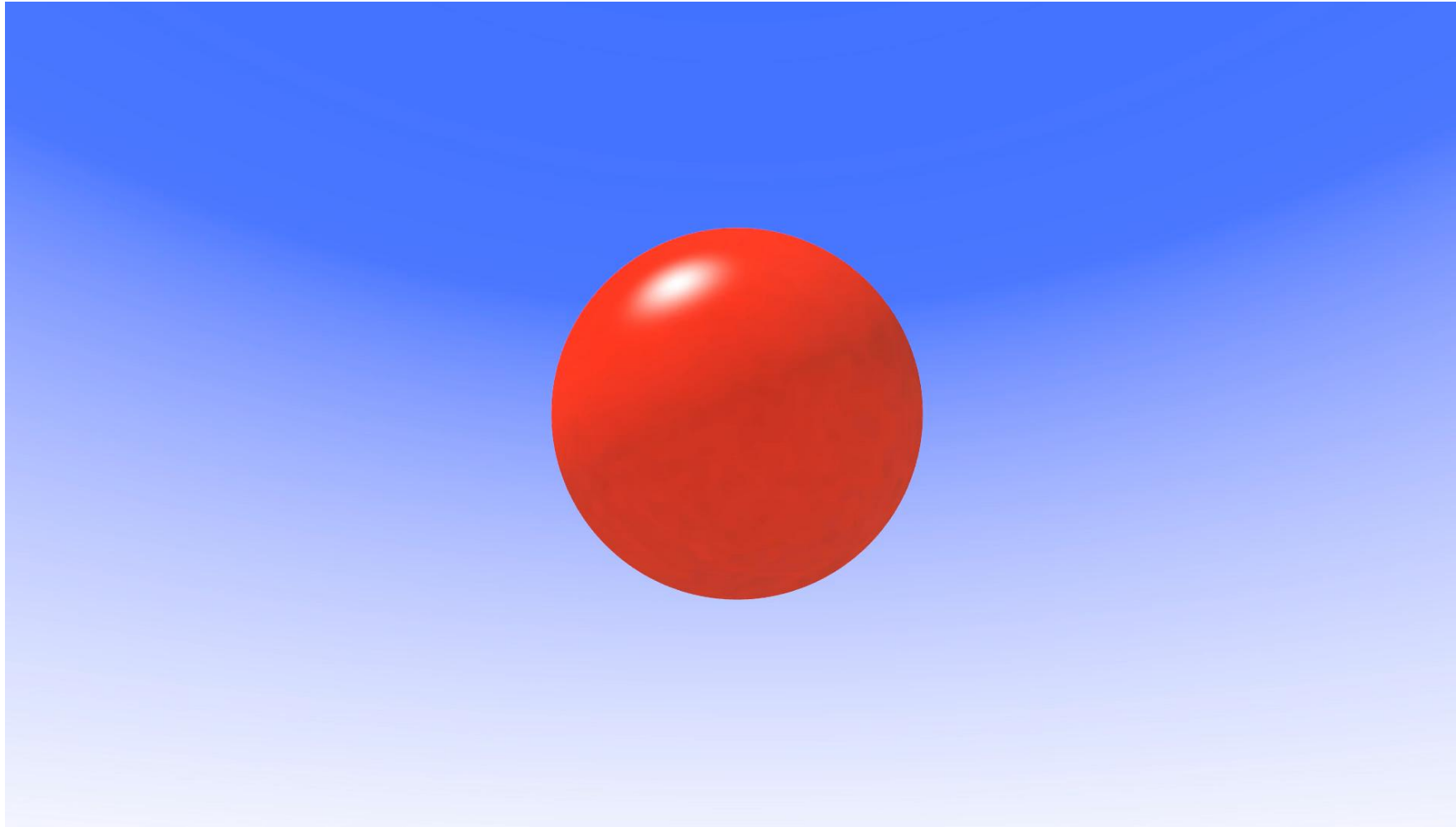


# Chrono:

## Support for Advanced Modeling Techniques

- Modeling; what does it mean?
  - The process of formulating a set of governing differential equations that captures the physics associated with the engineering problem of interest
- Modeling decisions are consequential
  - Hallmark of good modeling: it leads to a palatable math problem that can be solved numerically with relative ease

# Chrono::Flex - Dealing with Compliant Bodies



# Deformable Body Modeling Support in Chrono

## Equation of Motion & Mass Matrix

- Equations of Motion:

$$\mathbf{M}\ddot{\mathbf{e}} + \mathbf{Q}_s = \mathbf{Q}_e$$

- Mass matrix is constant and SPD

$$\mathbf{M} = \left[ \int_{V_o} \rho \mathbf{S}^T \mathbf{S} dV_o \right]$$

## System Forces

- Due to gravity

$$\mathbf{Q}_e = A \int_0^l \mathbf{S}^T \mathbf{f}_g dx$$

- Due to a concentrated force:

$$\mathbf{Q}_e = \mathbf{S}^T \mathbf{f}$$



# Deformable Bodies: Internal Forces...

- Strain Energy (shown for beam elements):

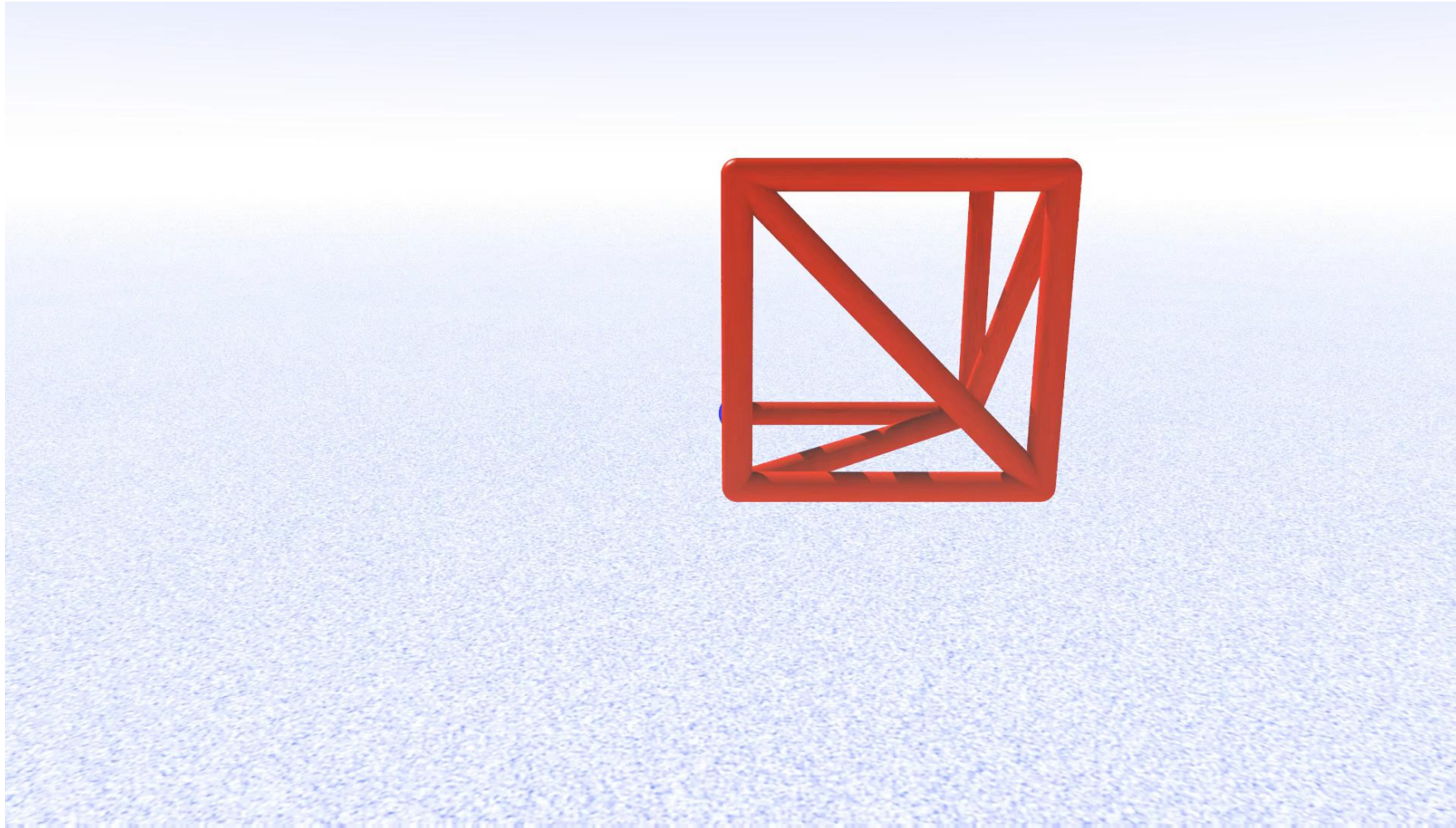
$$U = \frac{1}{2} \int_0^l EA(\varepsilon_{11})^2 dx + \frac{1}{2} \int_0^l EI(\kappa)^2 dx$$

- Partial Derivative of Strain Energy wrt generalized coordinated  $\mathbf{e}$  yields the Internal Forces

$$\mathbf{Q}_s = \int_0^l EA(\varepsilon_{11}) \left( \frac{\partial \varepsilon_{11}}{\partial \mathbf{e}} \right)^T dx + \int_0^l EI(\kappa) \left( \frac{\partial \kappa}{\partial \mathbf{e}} \right)^T dx$$

- Bad news: internal force expensive to evaluate
- Good News: for large systems can be done in parallel

# Deformable Bodies with Constraints



# Deformable Bodies with Constraints

- Constraints assumed holonomic, formulated as

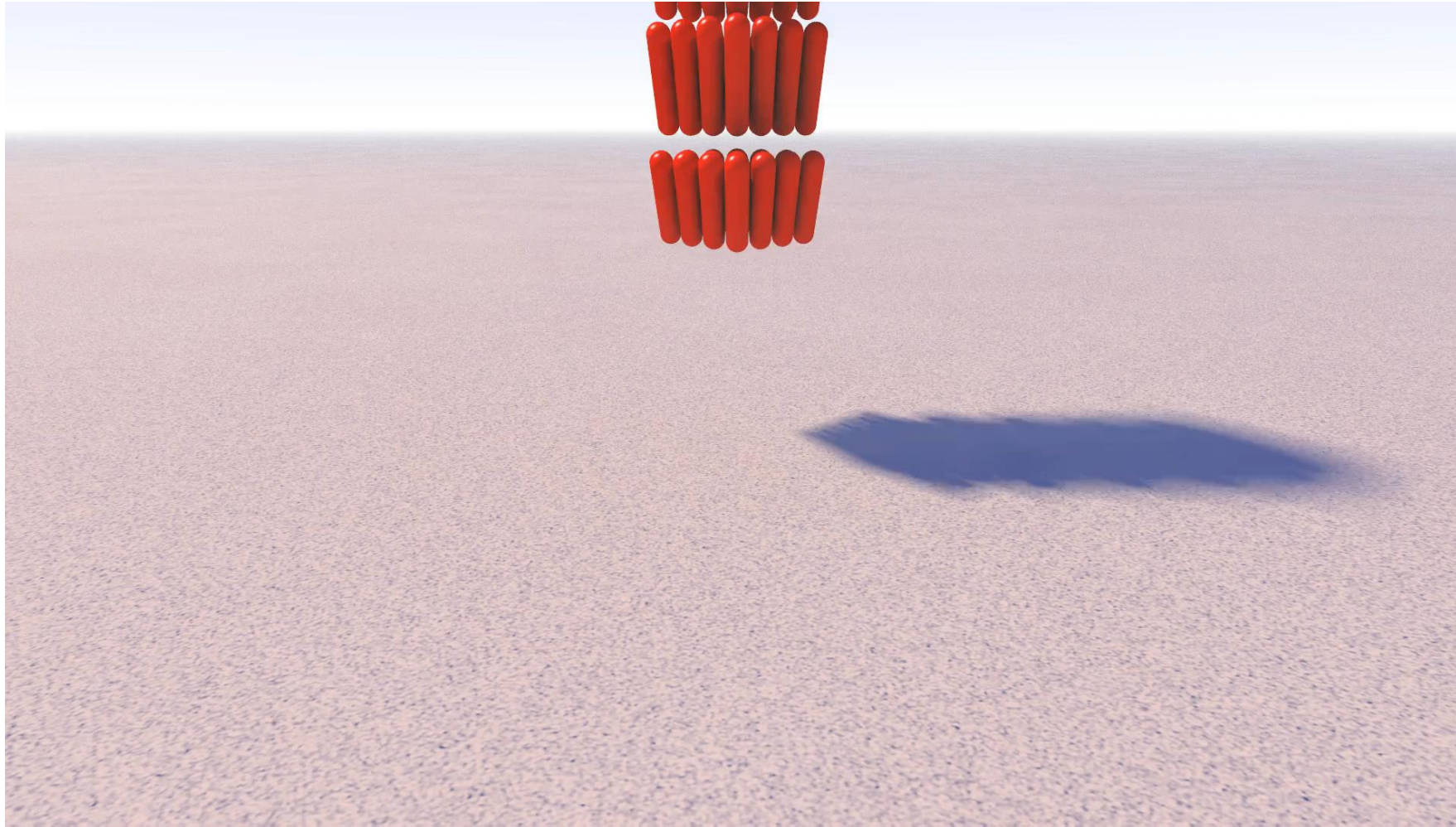
$$\Phi(\mathbf{q}, t) = [\Phi_1(\mathbf{q}, t) \dots \Phi_m(\mathbf{q}, t)]^T = 0$$

- Constraint form of the Equations of Motion (index 3 DAE problem)

$$\mathbf{M}\ddot{\mathbf{q}} + \Phi_{\mathbf{q}}^T(\mathbf{q}, t)\lambda + \mathbf{Q}_{\text{int}}(\mathbf{q}) = \mathbf{Q}_{\text{ext}}(\dot{\mathbf{q}}, \mathbf{q}, t)$$

# Wiggly Bodies

[Flexible bodies, w/ Friction and Contact: parallel simulation on the GPU]





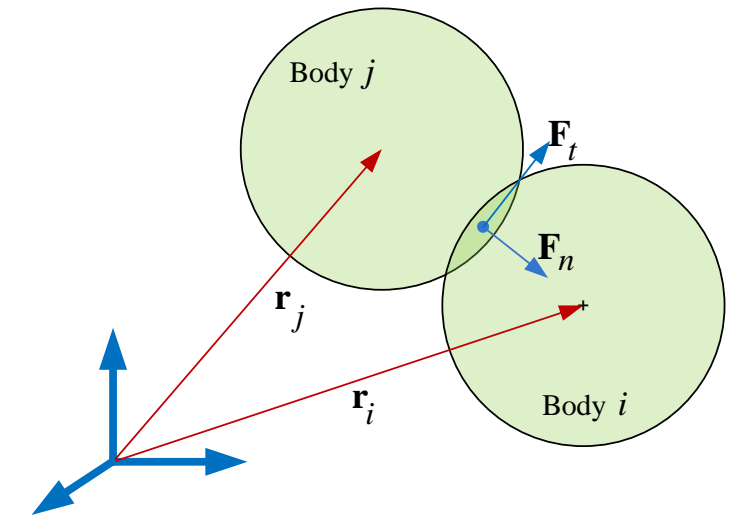
# Deformable Bodies with Friction and Contact

- Contact forces depend on several parameters:
  - Contact penetration
  - Normal vector
  - Relative velocity of colliding bodies at the point of contact
  - Etc.
- Normal force due to a collision calculated as

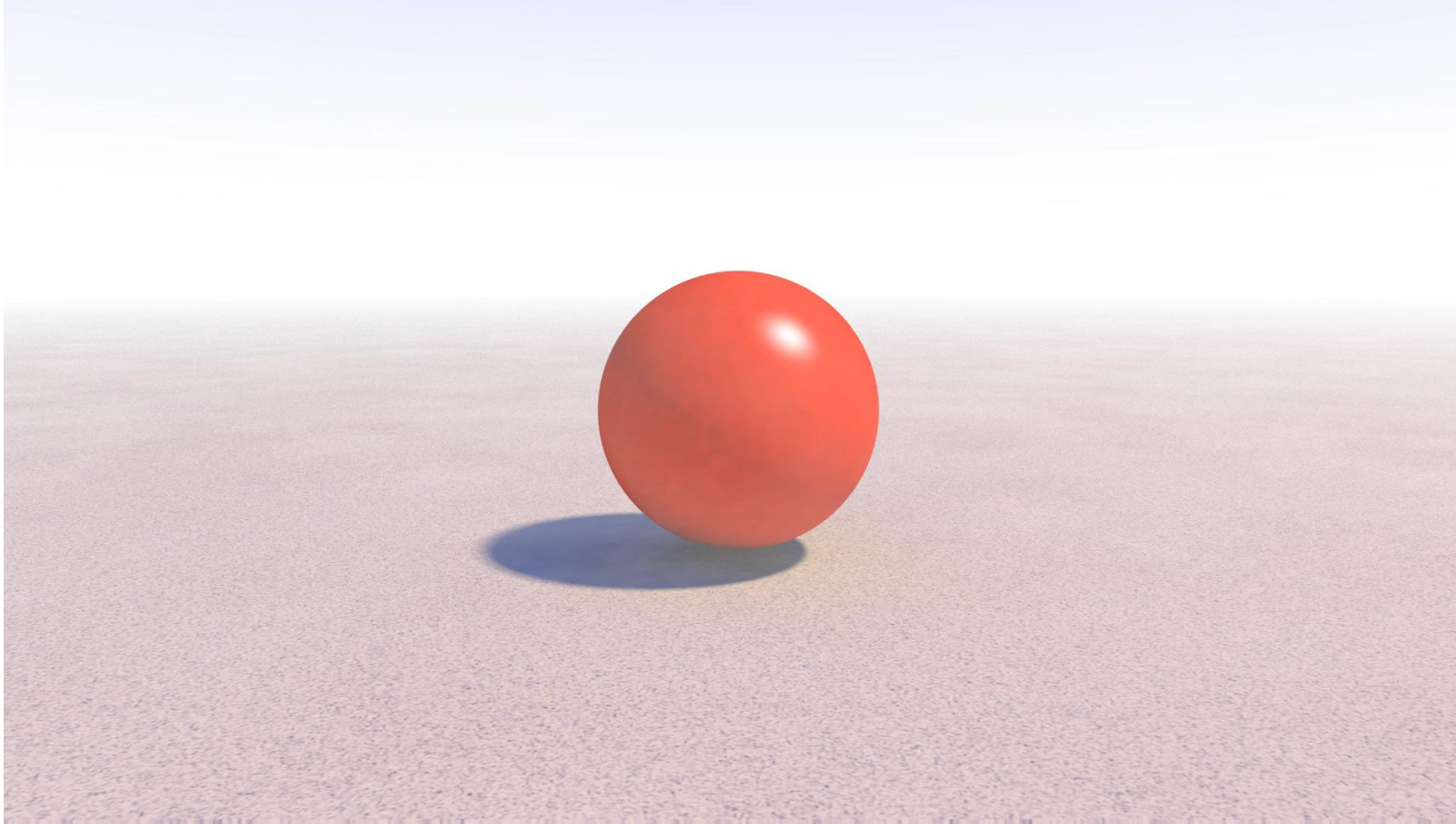
$$F_n = K\delta^n$$

$$K = \frac{4}{3(\sigma_i + \sigma_j)} \left[ \frac{R_i R_j}{R_i + R_j} \right]^{0.5}$$

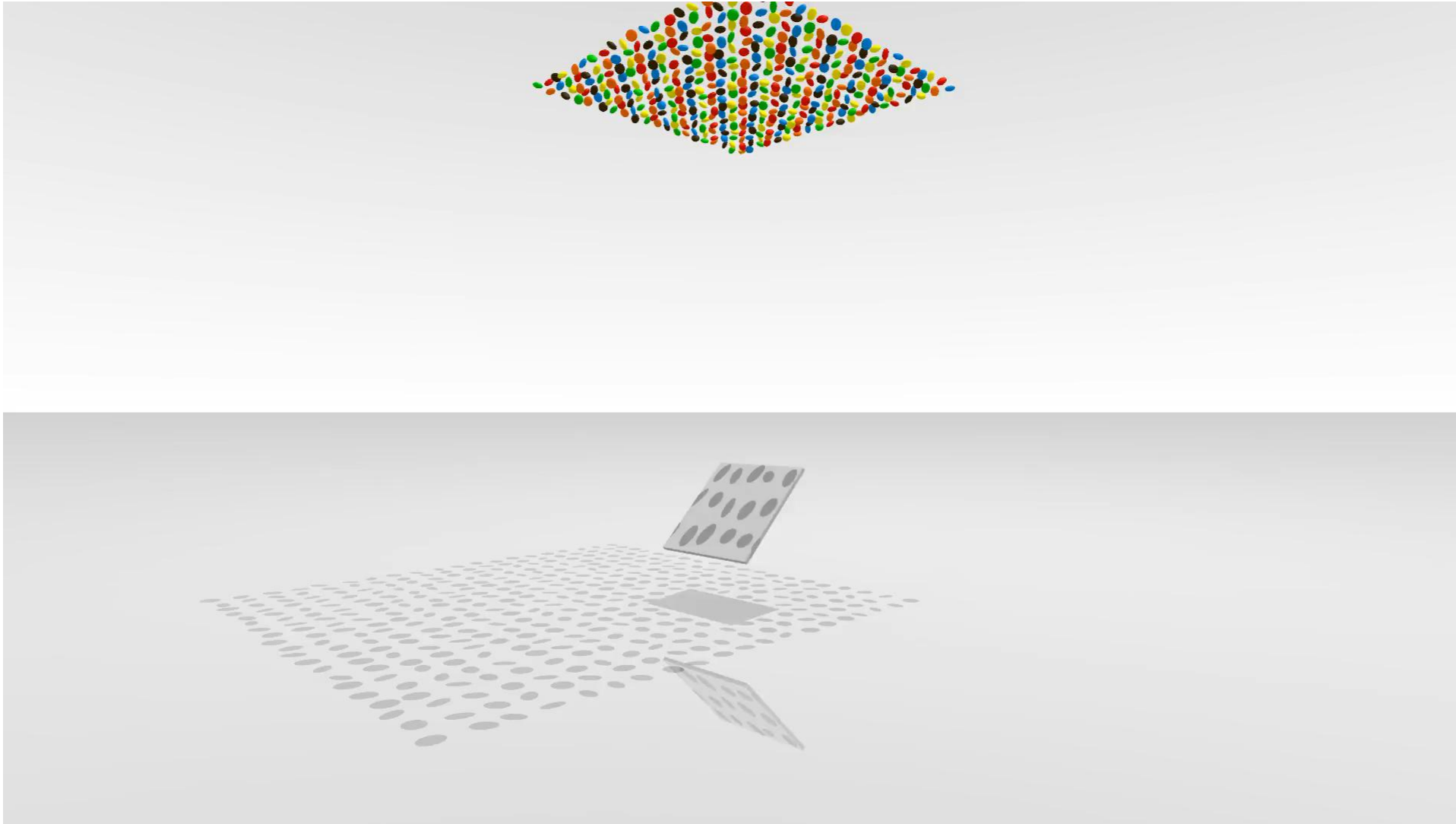
- Damping and friction can also be introduced
- Relies on a spherical decomposition of the geometry



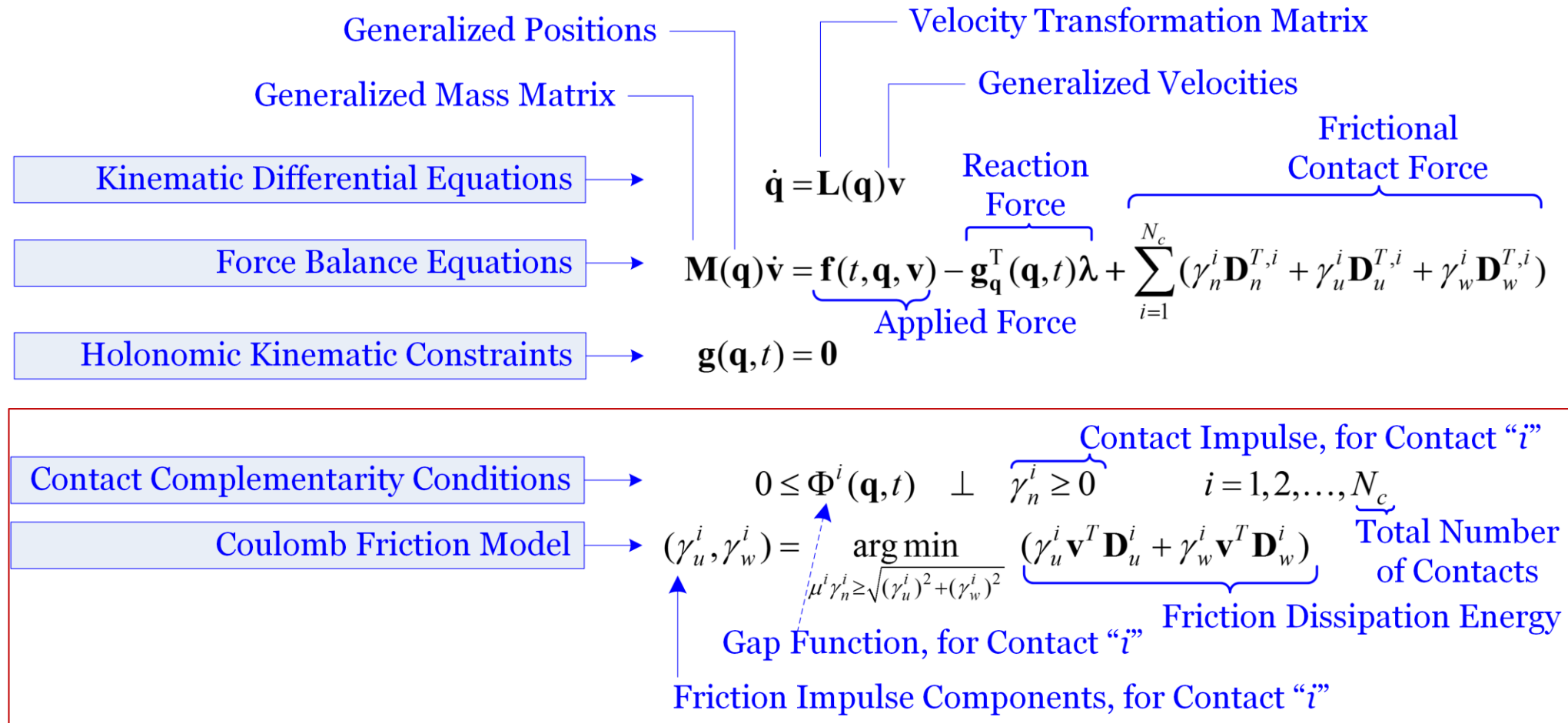
# Ball – Deformable Net Interaction



# Chrono::Rigid - Mixing 50,000 M&Ms on the GPU

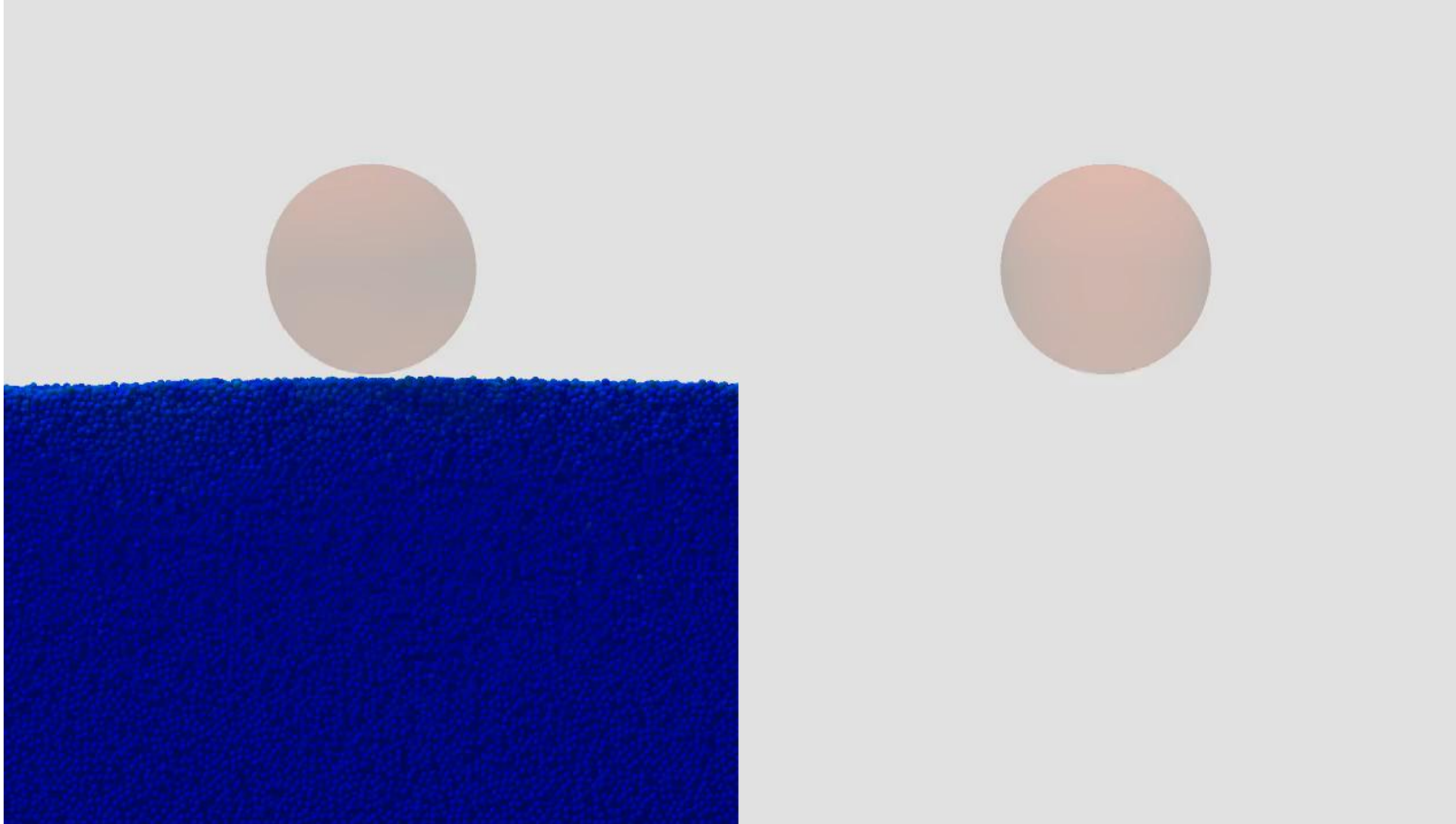


# Many-Body Dynamics with Friction and Contact

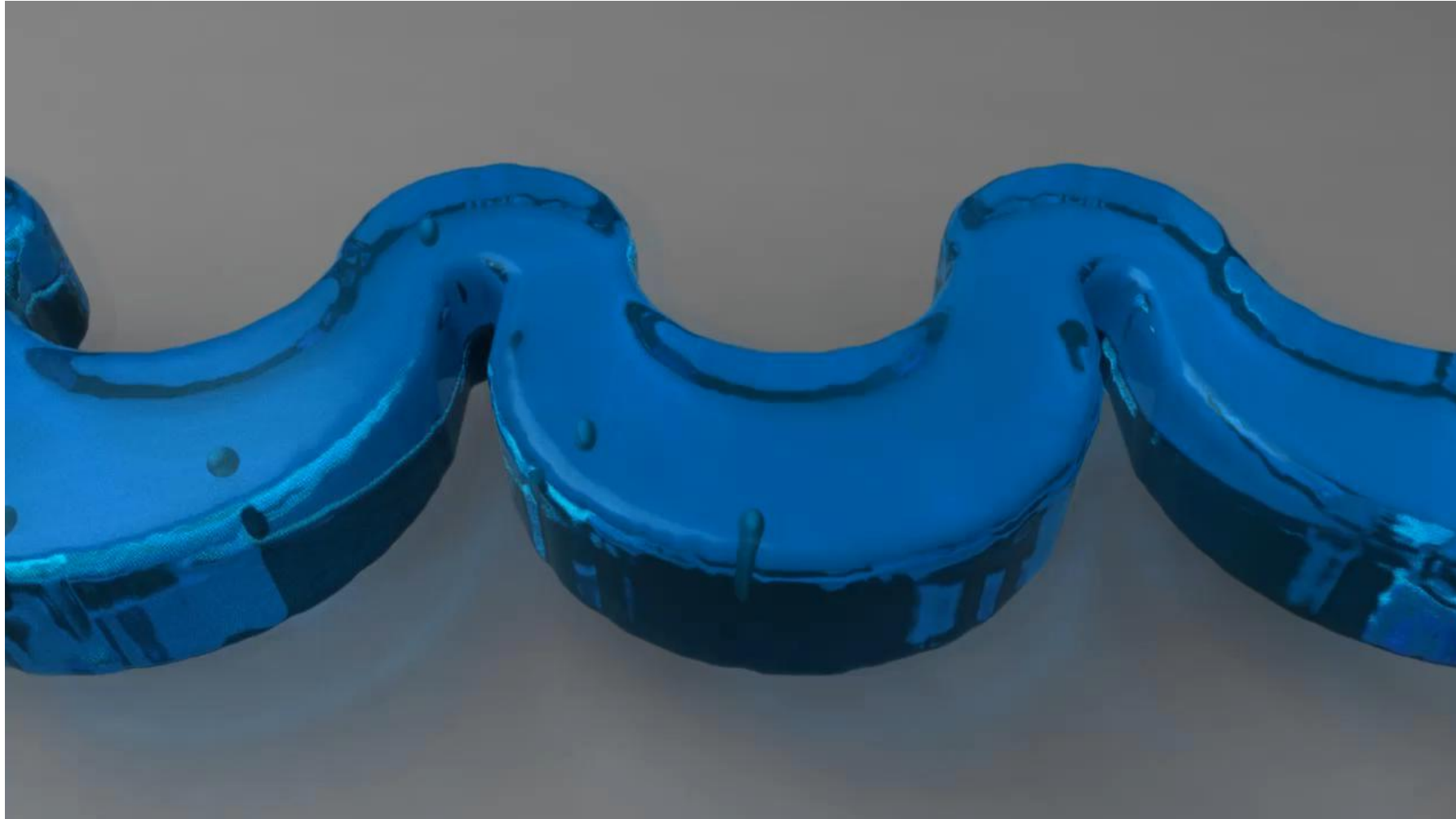




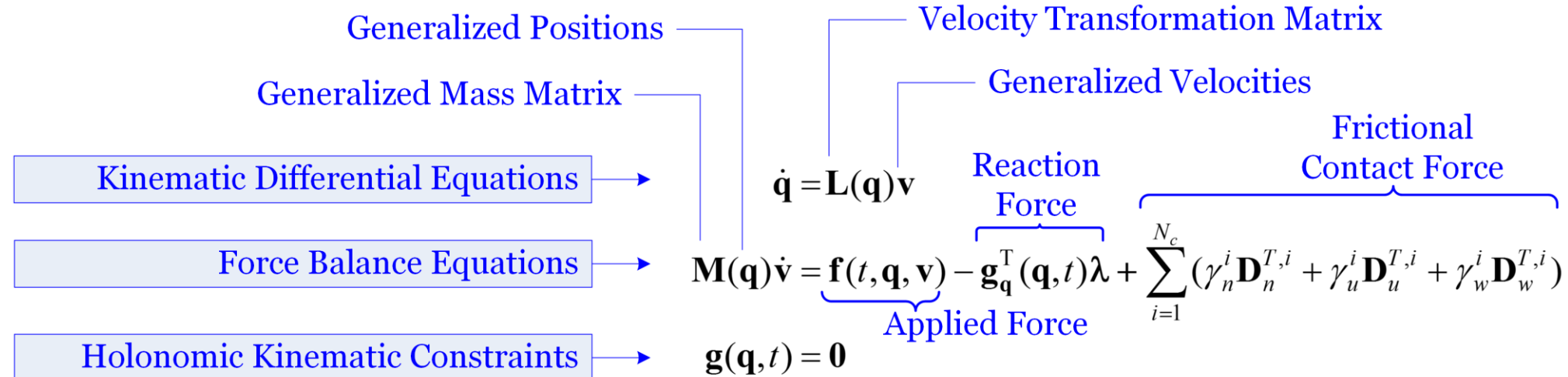
$h=10\text{ cm}, \rho_b=2.2\text{ g/cm}^3$



# Chrono::Flow Particle in Suspension Flow



# Coupled Problem: Fluid-Solid Interaction



Conservation of mass:

$$\frac{d\rho}{dt} = -\rho \frac{\partial v^\beta}{\partial x^\beta}$$

Conservation of momentum:

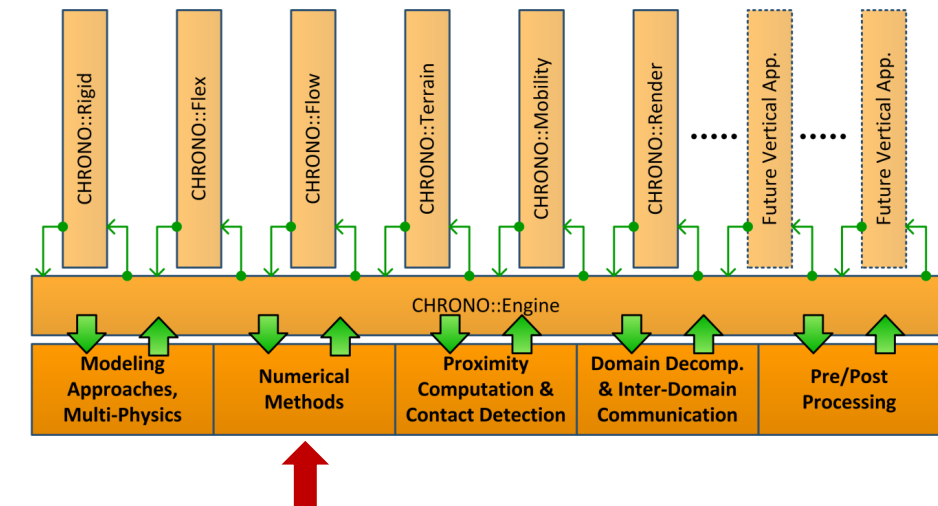
$$\frac{dv^\alpha}{dt} = \frac{1}{\rho} \frac{\partial \sigma^{\alpha\beta}}{\partial x^\beta} + \frac{f^\alpha}{\rho}$$

Conservation of energy:

$$\frac{du}{dt} = \frac{\sigma^{\alpha\beta}}{\rho} \frac{\partial v^\alpha}{\partial x^\beta}$$

# Algorithmic (applied math) support

Advanced modeling techniques  
 Algorithmic (applied math) support  
 Proximity computation  
 Domain decomposition & Inter-domain data exchange  
 Post-processing (visualization)



# Deformable Bodies: Implicit Integration using Newmark...

## Newmark Integration Formula

- New positions and velocities obtained at  $t_{n+1}$  based on new accelerations & Lagrange multipliers

$$\mathbf{q}_{n+1} = \mathbf{q}_n + h\dot{\mathbf{q}}_n + \frac{h^2}{2}[(1-2\beta)\ddot{\mathbf{q}}_n + 2\beta\ddot{\mathbf{q}}_{n+1}]$$

$$\dot{\mathbf{q}}_{n+1} = \dot{\mathbf{q}}_n + h[(1-\gamma)\ddot{\mathbf{q}}_n + \gamma\ddot{\mathbf{q}}_{n+1}]$$

## Index 3 DAE Problem

- Discretized Equations of Motion at  $t_{n+1}$ :

$$(\mathbf{M}\ddot{\mathbf{q}})_{n+1} + (\Phi_{\mathbf{q}}^T \boldsymbol{\lambda})_{n+1} + (\mathbf{Q}_{\text{int}} - \mathbf{Q}_{\text{ext}})_{n+1} = 0$$

- Kinematic constraints evaluated at new time step  $t_{n+1}$ :

$$\Phi(\mathbf{q}_{n+1}, t_{n+1}) = 0$$

# Deformable Bodies: Implicit Integration using Newmark...

- Solving an index 3 set of Differential Algebraic Equations (DAEs) w/ implicit integration
  - Relies on Newton-Krylov approach to solve nonlinear problem at each time step
  - Updates in the accelerations at iteration (k) computed as

$$\begin{bmatrix} \hat{\mathbf{M}} & \Phi_{\mathbf{q}}^T \\ \Phi_{\mathbf{q}} & \mathbf{0} \end{bmatrix} \begin{bmatrix} \Delta \ddot{\mathbf{q}} \\ \Delta \lambda \end{bmatrix}^{(k)} = \begin{bmatrix} -\mathbf{e}_1 \\ -\mathbf{e}_2 \end{bmatrix}^{(k)}$$

- Residuals capture error in satisfying the equations of motion and the kinematic constraint equations:

$$\mathbf{e}_1 = (\mathbf{M}\ddot{\mathbf{q}})_{n+1} + (\Phi_{\mathbf{q}}^T \lambda)_{n+1} + (\mathbf{Q}_{\text{int}})_{n+1} - (\mathbf{Q}_{\text{ext}})_{n+1}$$

$$\mathbf{e}_2 = \frac{1}{\beta h^2} \Phi(\mathbf{q}_{n+1}, t_{n+1})$$

# Jacobian Matrix Computation, Flex Body Dynamics

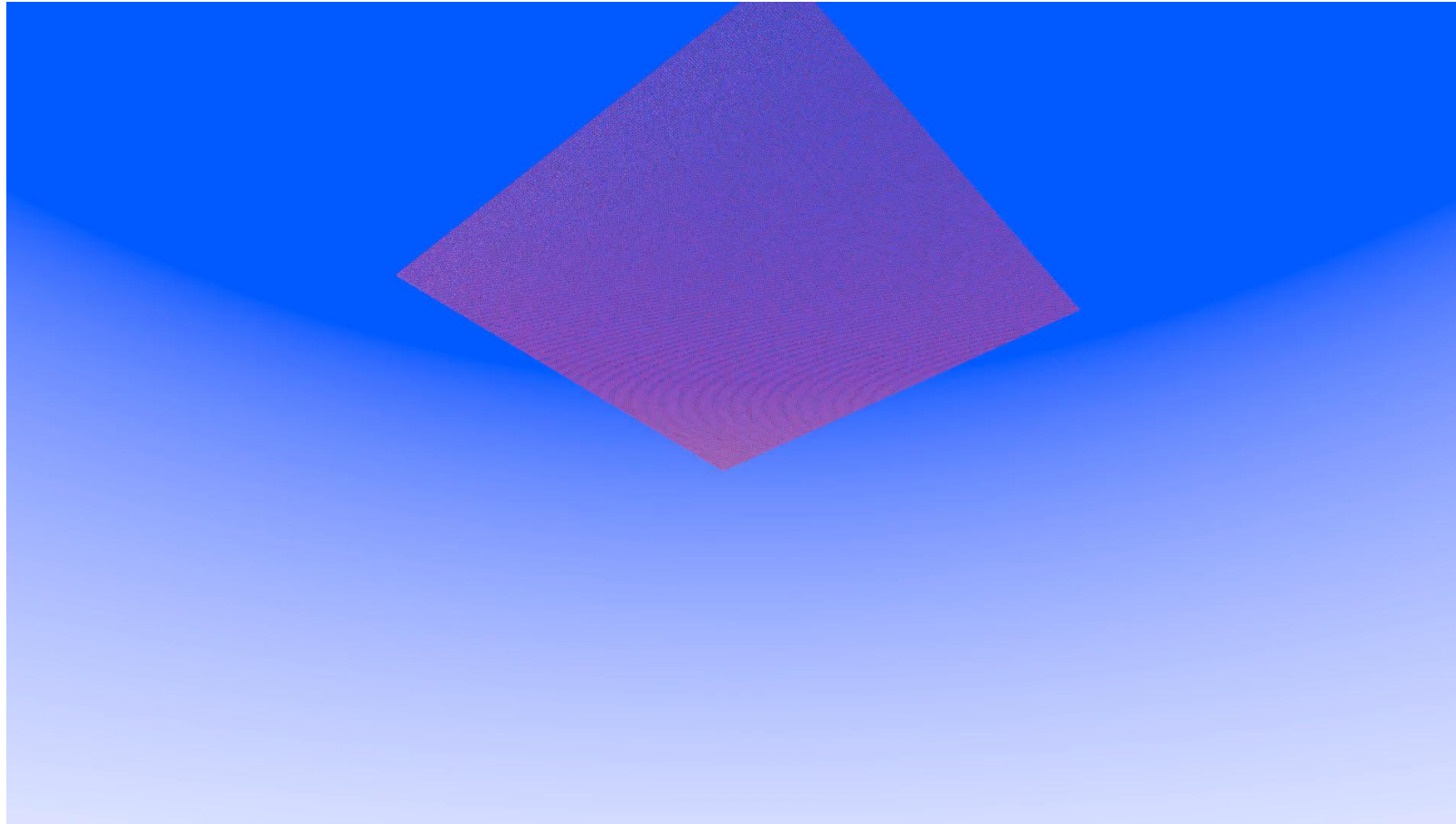
- Sensitivity computation costly

$$\hat{\mathbf{M}} = \frac{\partial \mathbf{e}_1}{\partial \ddot{\mathbf{q}}} = \mathbf{M} - h\gamma \left[ \frac{\partial \mathbf{Q}_{ext}}{\partial \dot{\mathbf{q}}} \right] + \beta h^2 \left[ (\Phi_q^T \lambda)_q + \frac{\partial \mathbf{Q}_{int}}{\partial \mathbf{q}} - \frac{\partial \mathbf{Q}_{ext}}{\partial \mathbf{q}} \right]$$

- Computational bottleneck is evaluation of sensitivity of internal forces:

$$\frac{\partial \mathbf{Q}_{int}}{\partial \mathbf{q}} = \int_0^l EA(\varepsilon_{11}) \frac{\partial}{\partial \mathbf{e}} \left( \frac{\partial \varepsilon_{11}}{\partial \mathbf{e}} \right)^T dx + \int_0^l EA \left( \frac{\partial \varepsilon_{11}}{\partial \mathbf{e}} \right)^T \left( \frac{\partial \varepsilon_{11}}{\partial \mathbf{e}} \right) dx + \int_0^l EI(\kappa) \frac{\partial}{\partial \mathbf{e}} \left( \frac{\partial \kappa}{\partial \mathbf{e}} \right)^T dx + \int_0^l EI \left( \frac{\partial \kappa}{\partial \mathbf{e}} \right)^T \left( \frac{\partial \kappa}{\partial \mathbf{e}} \right) dx$$

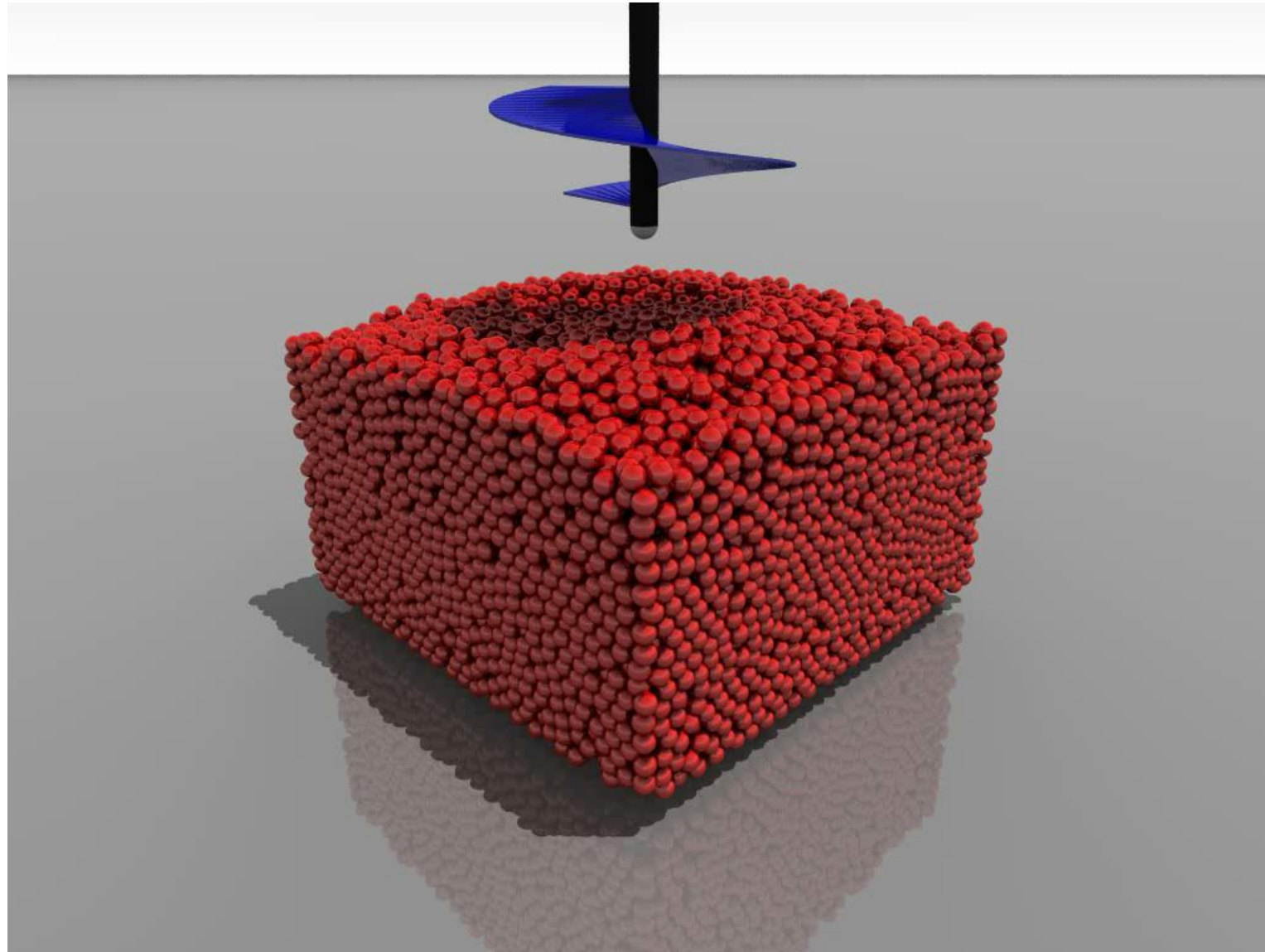
# 0.25 km Net Simulation: 101,025 Beams & 640,146 Constraints



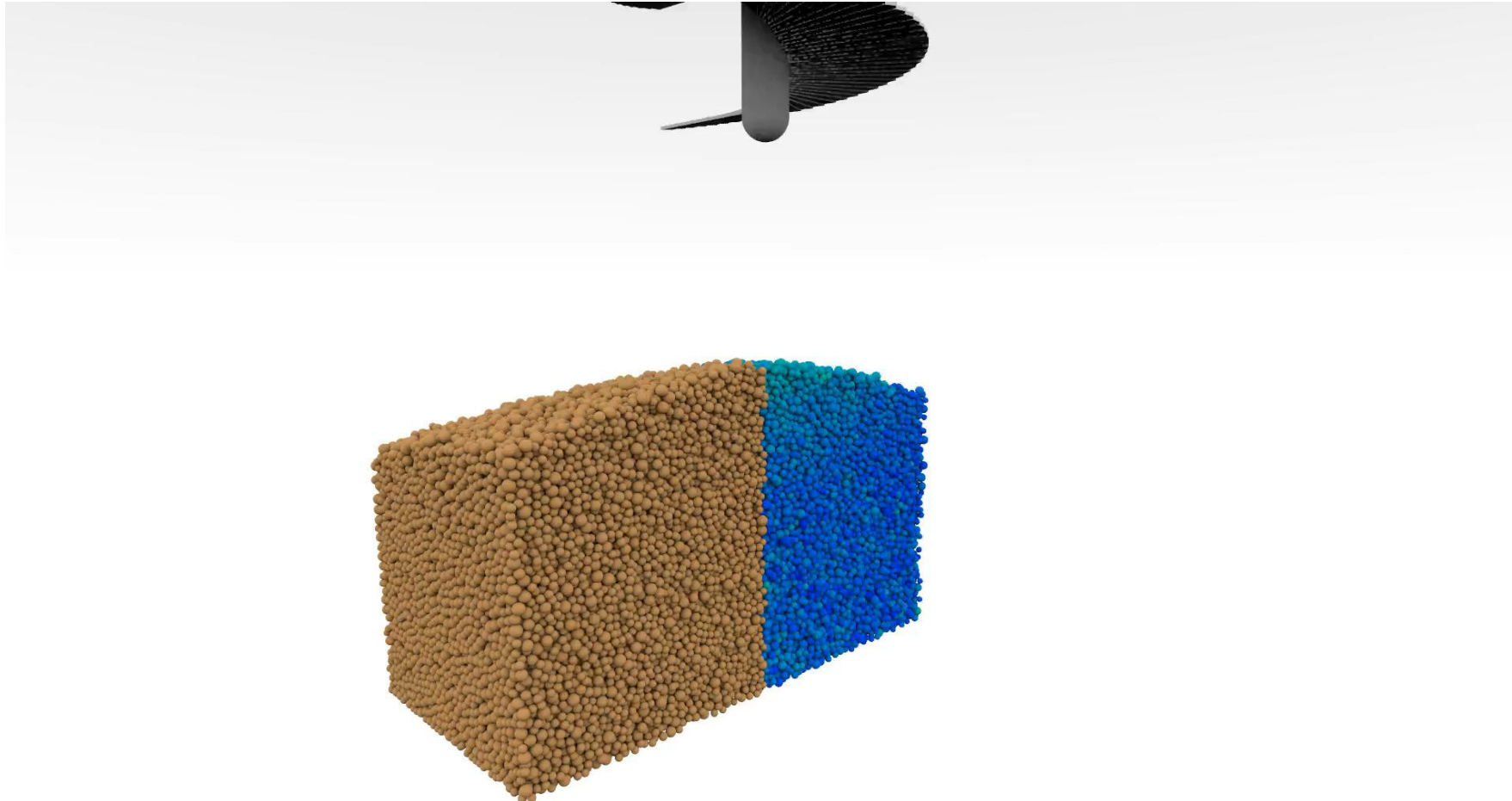


# 200,000 Bodies & 10 kg Anchor

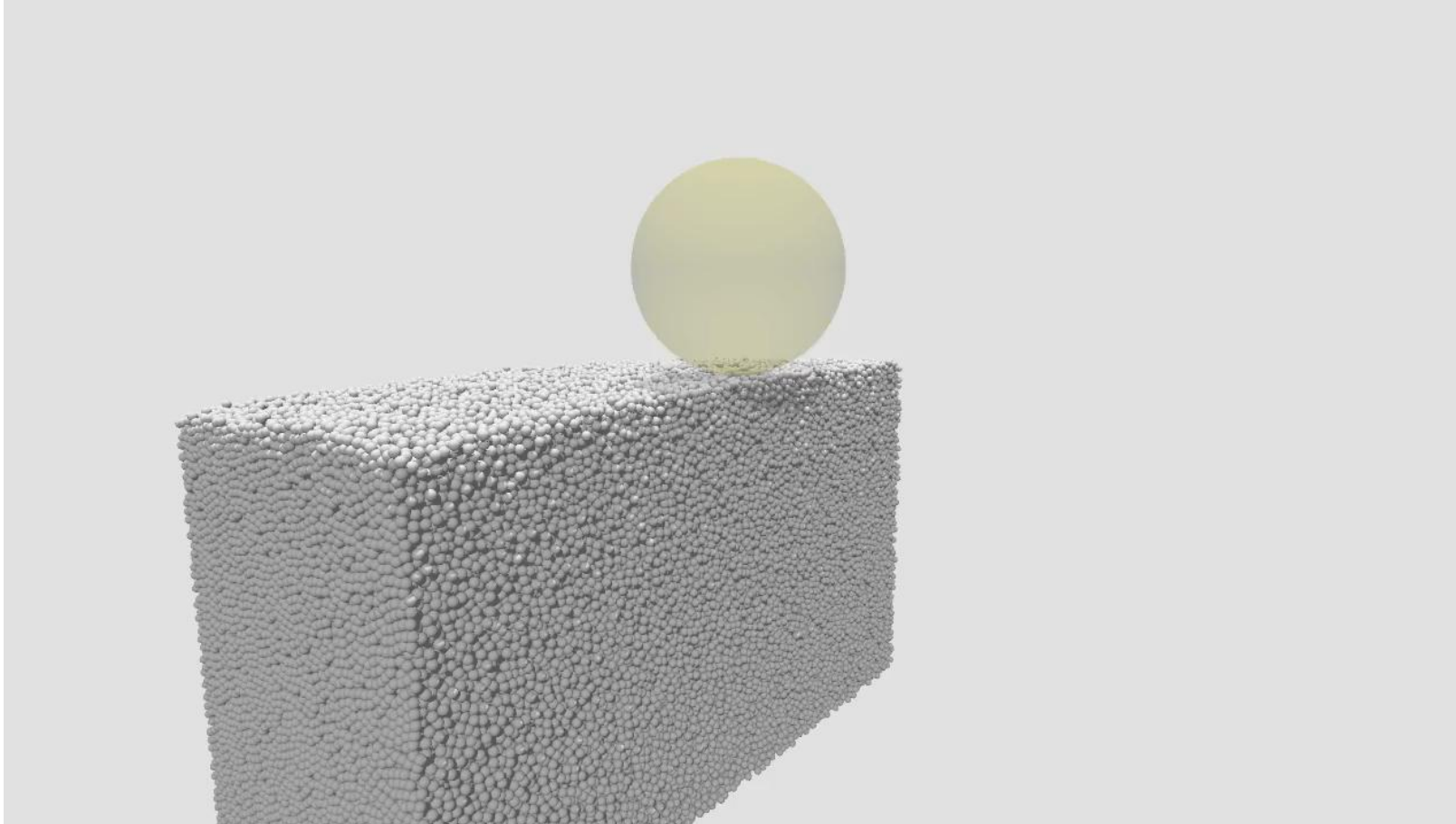
[solved in parallel on the GPU]



# Cut-away, Anchoring Simulation



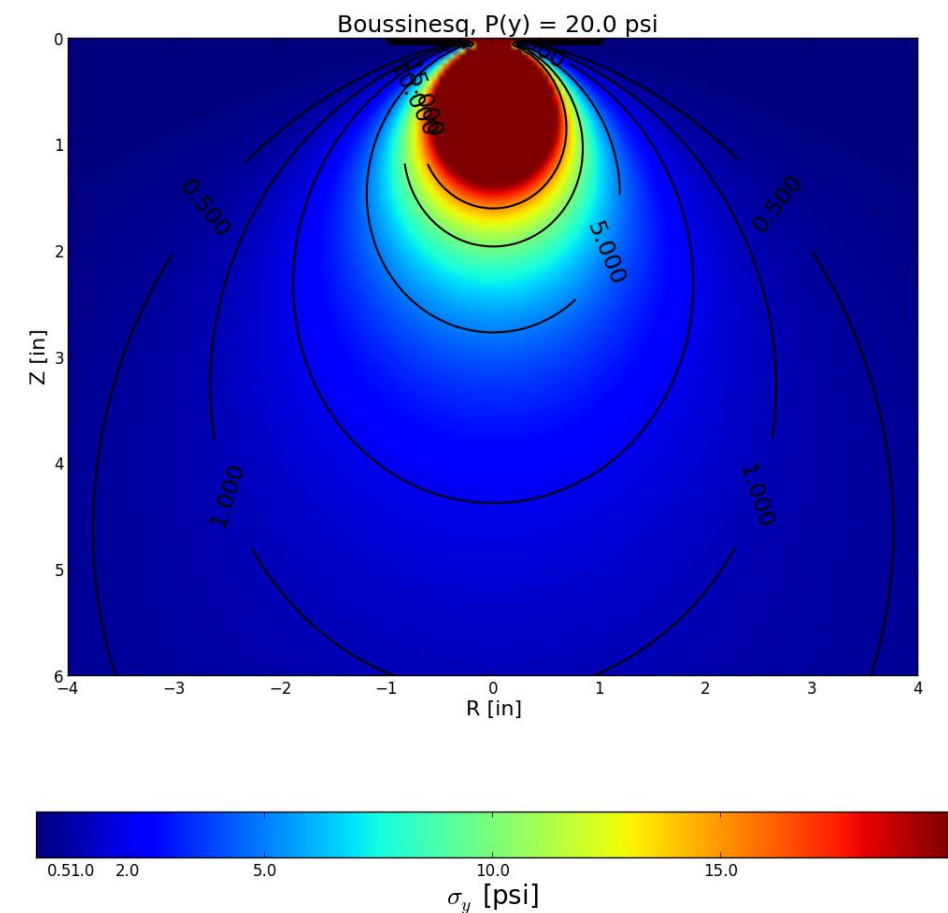
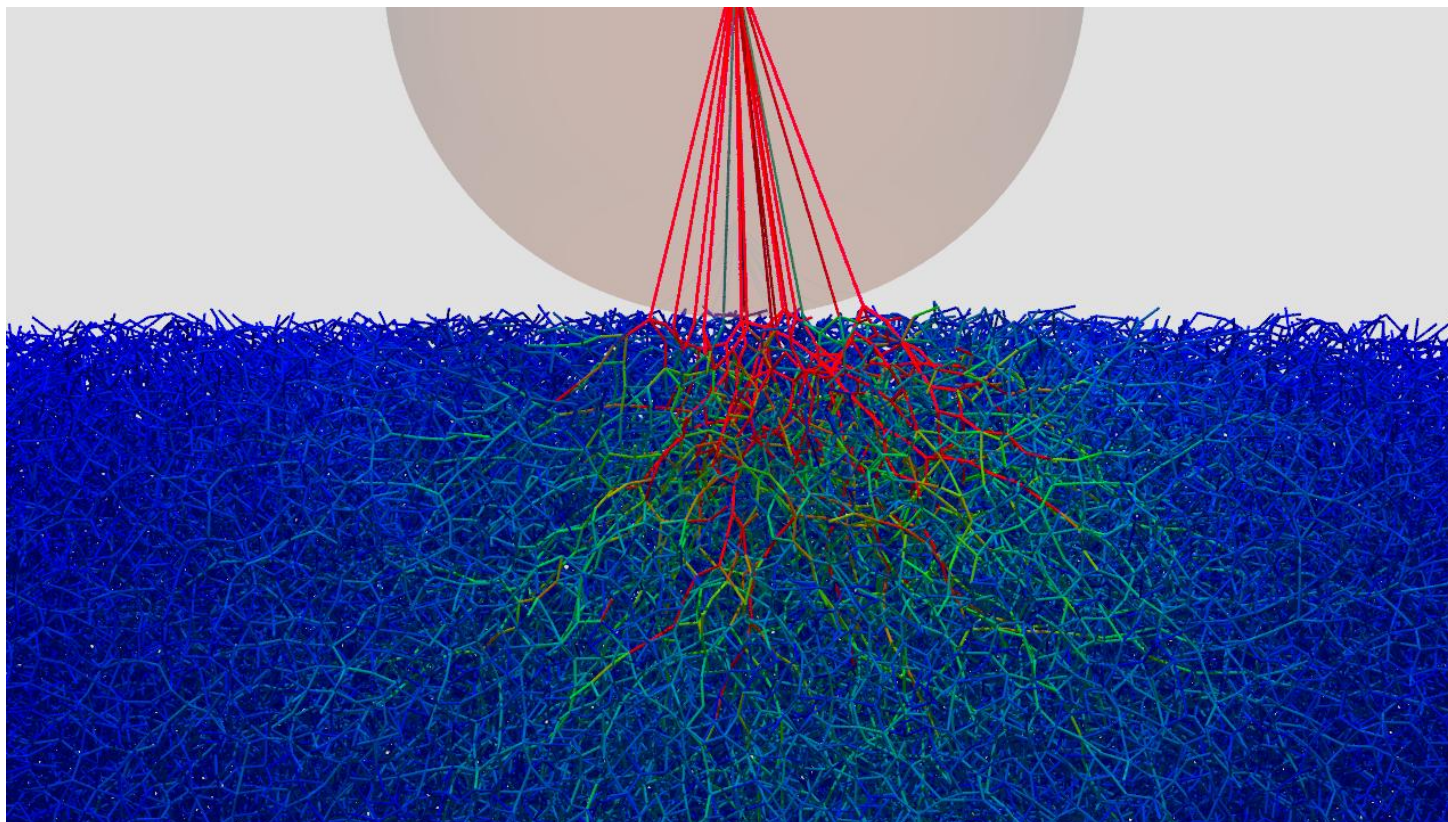
# 0.5 Million Rigid Bodies





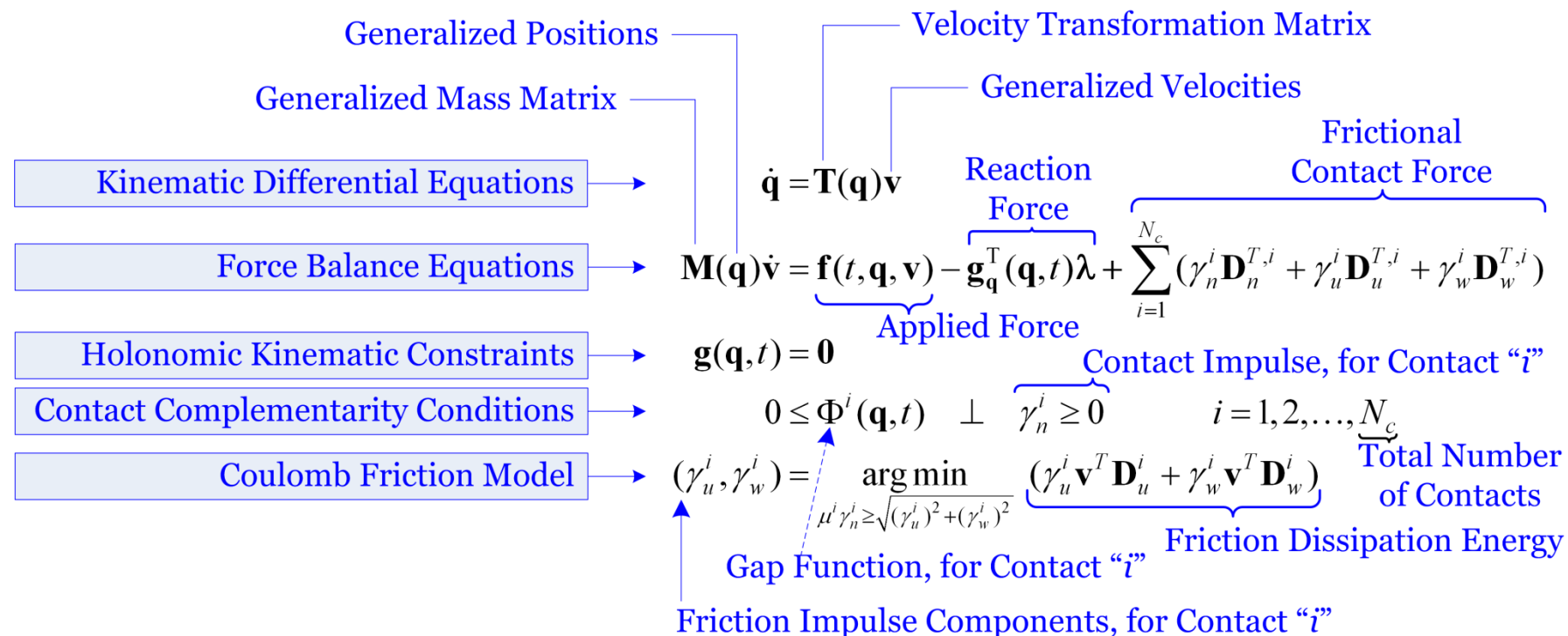
# 0.5 Million Rigid Bodies

- Granular material has unique properties



# Rigid Body Dynamics w/ DVI: From Continuum to Discrete

- Seeking to solve numerically the equations of motion robustly & effectively
- Discussion focused here on many-body dynamics



# The Discretized Problem: from $t_l$ to $t_{l+1}$

positions time step index

$$\mathbf{q}^{(l+1)} = \mathbf{q}^{(l)} + h\mathbf{L}(\mathbf{q}^{(l)})\mathbf{v}^{(l+1)}$$

Mass Mat. speeds Applied Forces Reaction impulses

$$\mathbf{M}(\mathbf{v}^{(l+1)} - \mathbf{v}^l) = hf(t^{(l)}, \mathbf{q}^{(l)}, \mathbf{v}^{(l)}) + \sum_{i \in \mathcal{A}(q^{(l)}, \delta)} (\gamma_{i,n} \mathbf{D}_{i,n} + \gamma_{i,u} \mathbf{D}_{i,u} + \gamma_{i,w} \mathbf{D}_{i,w})$$

$i \in \mathcal{A}(q^{(l)}, \delta) :$   $0 \leq \frac{1}{h} \Phi_i(\mathbf{q}^{(l)}) + \mathbf{D}_{i,n}^T \mathbf{v}^{(l+1)} \perp \gamma_n^i \geq 0,$  Complementarity Condition

$(\gamma_{i,u}, \gamma_{i,w}) = \underset{\mu_i \gamma_{i,n} \geq \sqrt{\gamma_{i,u}^2 + \gamma_{i,w}^2}}{\operatorname{argmin}} \mathbf{v}^T (\gamma_{i,u} \mathbf{D}_{i,u} + \gamma_{i,w} \mathbf{D}_{i,w}).$  Coulomb 3D friction model

Stabilization term

(D. Stewart, 1998)

# The Cone Complementarity Problem (CCP)

- Define the convex hypercone...

$$\Upsilon = \left( \bigoplus_{i \in \mathcal{A}(\mathbf{q}^l, \epsilon)} \mathcal{FC}^i \right)$$

$\mathcal{FC}^i \in \mathbb{R}^3$  represents friction cone associated with  $i^{th}$  contact

- ... and its polar hypercone:

$$\Upsilon^\circ = \left( \bigoplus_{i \in \mathcal{A}(\mathbf{q}^l, \epsilon)} \mathcal{FC}^{i^\circ} \right)$$

- The problem can be formulated as find  $\gamma$  that solves the following CCP

$$\gamma \in \Upsilon \perp -(\mathbf{N}\gamma + \mathbf{d}) \in \Upsilon^\circ$$



# The Quadratic Programming Angle...

- The CCP captures the first-order optimality condition for a quadratic optimization problem with conic constraints:

$$\begin{cases} \min \mathbf{q}(\gamma) = \frac{1}{2}\gamma^{\mathbf{T}}\mathbf{N}\gamma + \mathbf{d}^{\mathbf{T}}\gamma \\ \text{subject to } \gamma_i \in \Upsilon_i \text{ for } i = 1, 2, \dots, N_c \end{cases}$$

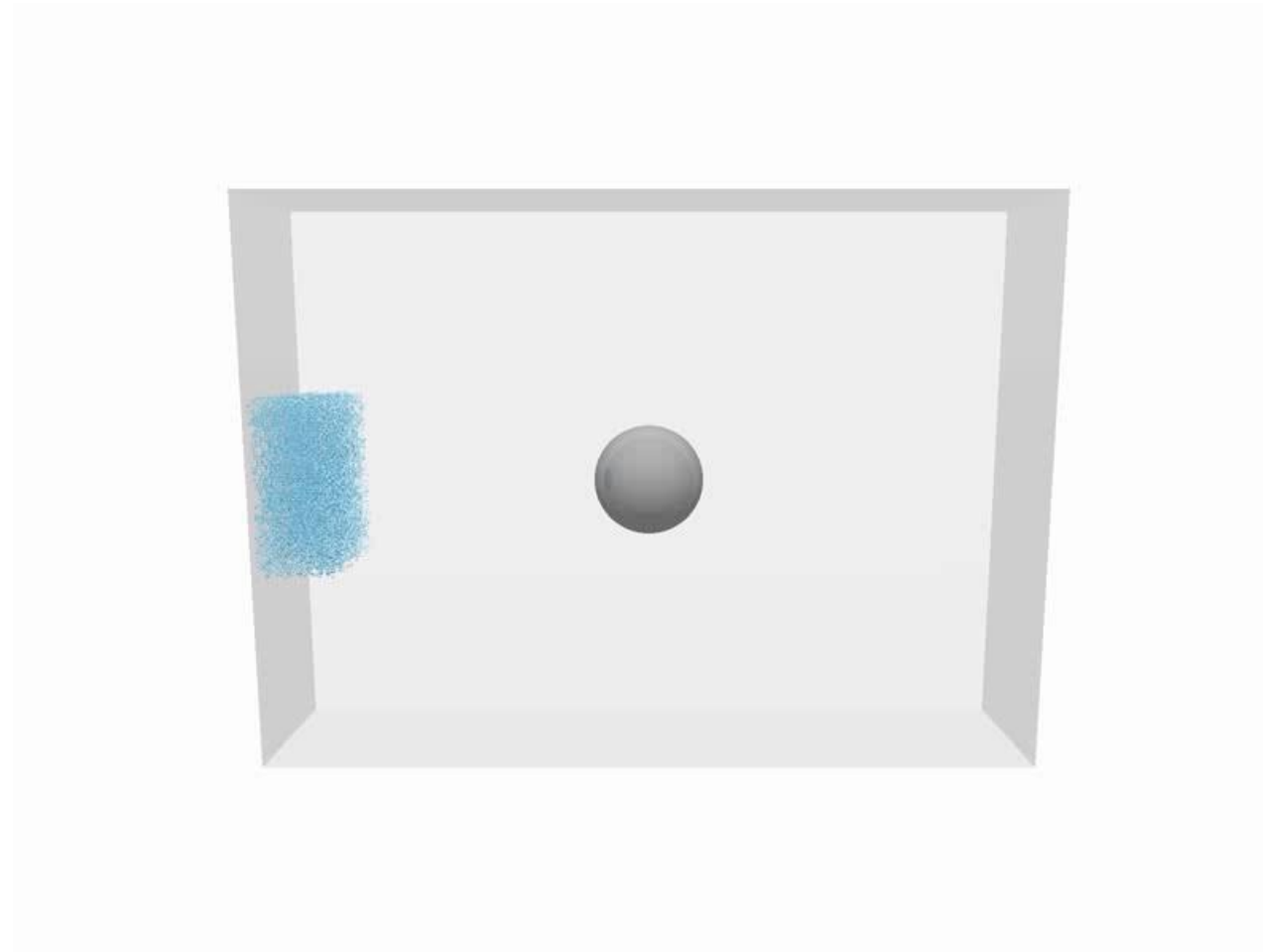
- Notation used:

$$\gamma \equiv [\gamma_1^T, \gamma_2^T, \dots, \gamma_{N_c}^T]^T \in \mathbb{R}^{3 \times N_c} \quad \text{and} \quad \Upsilon_i : (\gamma_{u,i}^2 + \gamma_{w,i}^2) - \mu_i^2 \gamma_{n,i}^2 \leq 0$$



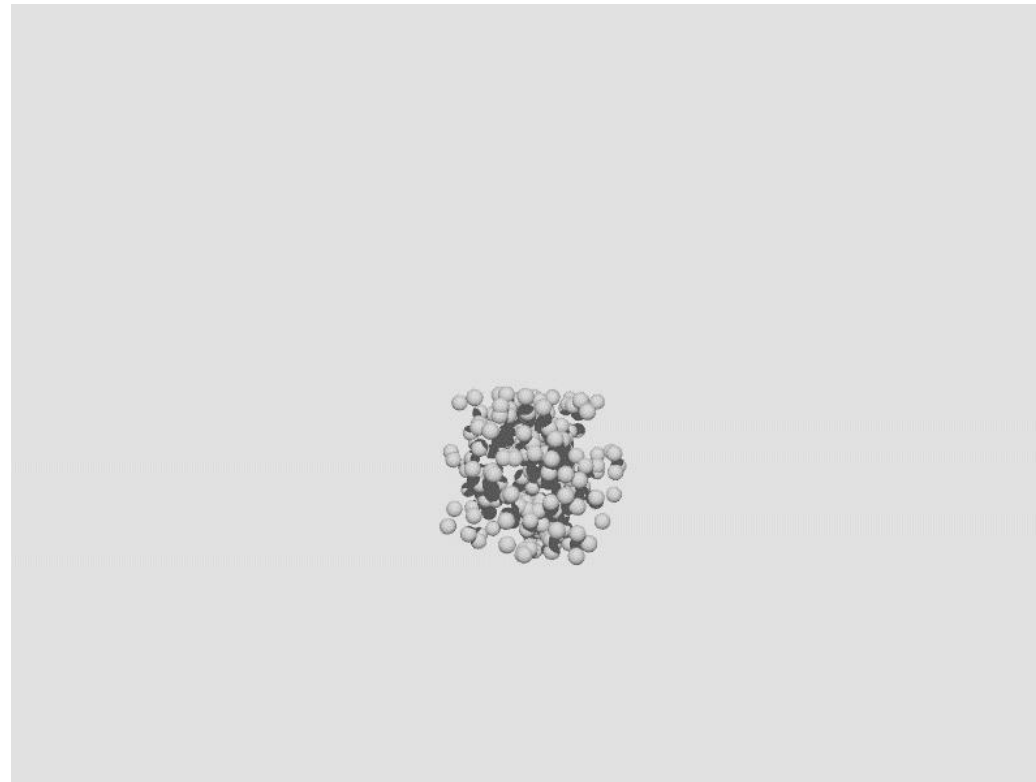
# 1 Million Rigid Spheres

[parallel on the GPU]

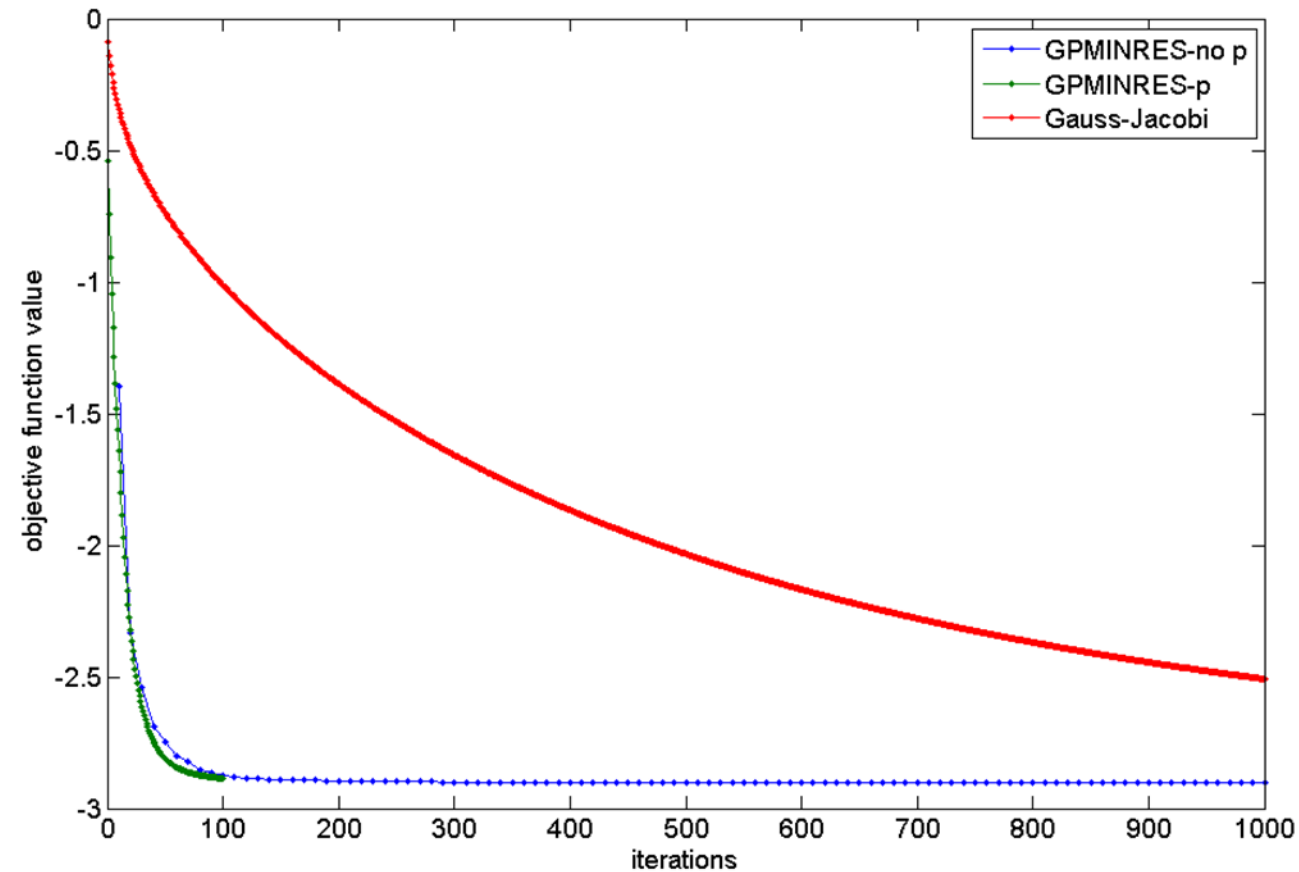


# Test Problem: 1000 rigid spheres with 3525 contacts

- Cost function depends on 3,525 variables (or about 10,500 if friction is present)



# Objective Function Value [1K bodies, 3525 contacts]



# Jacobi

$$\begin{aligned}\tilde{\gamma}^{r+1} &= \gamma^r + \omega \mathbf{B}[\mathbf{N}\gamma^r + \mathbf{r}] \\ \hat{\gamma}^{r+1} &= \mathbb{P}(\tilde{\gamma}^{r+1}) \\ \gamma^{r+1} &= \lambda \hat{\gamma}^{r+1} + (1 - \lambda)\gamma^r .\end{aligned}$$

$$\mathbf{B} = \begin{bmatrix} \eta_1 & & \mathbf{0} \\ & \ddots & \\ \mathbf{0} & & \eta_{n_c} \end{bmatrix} ,$$

$$\eta_i = \frac{1}{\text{Trace}(\mathbf{D}_i^T \mathbf{M}^{-1} \mathbf{D}_i)} .$$

# GP-MINRES

ALGORITHM GPMINRES( $\mathbf{N}$ ,  $\mathbf{r}$ ,  $\tau$ ,  $\eta_1$ ,  $\eta_2$ ,  $N_{max}$ ,  $M_{max}$ )

```

(1)    $\gamma^{(0)} := \mathbf{0}_{nc}$ 
(2)   for  $k := 0$  to  $N_{max}$ 
(3)        $\mathbf{y}^{(0)} = \gamma^{(k)}$ 
(4)       while aggressively changing active set and reducing cost function
(5)            $\mathbf{y}^{(j+1)} = P[\mathbf{y}^{(j)} - \alpha_j \nabla q(\mathbf{y}^{(j)})]$ 
(6)            $j = j + 1$ 
(7)       endwhile
(8)        $\gamma^{(k)} := \mathbf{y}^{(j)}$ 
(9)       Determine active set  $\mathcal{A}(\gamma^{(k)})$  and  $\mathbf{Z}_k$  and  $\mathbf{r}_k$ 
(10)       $\mathbf{w}_0 = \mathbf{0}_{m_k}$ 
(11)      for  $j := 0$  to  $M_{max}$ 
(12)          MINRES step:  $\mathbf{w}^{(j)} \rightarrow \mathbf{w}^{(j+1)}$ 
(13)           $j = j + 1$ 
(14)          if slughish convergence
(15)              break
(16)      enfor
(17)      Set  $\bar{\mathbf{w}}_k := \mathbf{w}^{(j)}$ 
(18)      Get  $\gamma^{(k+1)} \rightarrow$  backtracking line-search with direction  $\mathbf{d}_k = \mathbf{Z}_k \bar{\mathbf{w}}_k$ 
(19)      if  $\|\nabla_{\Omega} q(\gamma^{(k+1)})\|_{\infty} < \tau$ 
(20)          break
(21)      enfor
(22)      return Value at time step  $t_{l+1}$ ,  $\gamma^{l+1} := \gamma^{(k+1)}$  .
    
```



# P-SPG-FB

ALGORITHM P-SPG-FB( $\mathbf{N}$ ,  $\mathbf{r}$ ,  $\mathbf{x}_0$ ,  $\mathcal{K}$ ,  $\mathbf{P} \mapsto \mathbf{x}$ )

- (1)  $\mathbf{x}_0 := \Pi_{\mathcal{K}}(\mathbf{x}_0)$ ,  $\mathbf{x}_{FB} = \mathbf{x}_0$ ,  $\hat{\alpha}_0 \in [\alpha_{min}, \alpha_{max}]$
- (2)  $\mathbf{g}_0 := \mathbf{N}\mathbf{x}_0 + \mathbf{r}$ ,  $f(\mathbf{x}_0) = \frac{1}{2}\mathbf{x}_0^T \mathbf{N}\mathbf{x}_0 + \mathbf{x}_0^T \mathbf{r}$ ,  $w_0 = 10^{29}$
- (3) **for**  $j := 0$  **to**  $N_{max}$
- (4)      $\mathbf{p}_j = \mathbf{P}^{-1}\mathbf{g}_j$
- (5)      $\mathbf{d}_j = \Pi_{\mathcal{K}}(\mathbf{x}_j - \hat{\alpha}_j\mathbf{p}_j) - \mathbf{x}_j$
- (6)     **if**  $\langle \mathbf{d}_j, \mathbf{g}_j \rangle \geq 0$
- (7)          $\mathbf{d}_j = \Pi_{\mathcal{K}}(\mathbf{x}_j - \hat{\alpha}_j\mathbf{g}_j) - \mathbf{x}_j$
- (8)      $\lambda := 1$
- (9)     **while** line search
- (10)          $\mathbf{x}_{j+1} := \mathbf{x}_j + \lambda\mathbf{d}_j$
- (11)          $\mathbf{g}_{j+1} := \mathbf{N}\mathbf{x}_{j+1} + \mathbf{r}$
- (12)          $f(\mathbf{x}_{j+1}) = \frac{1}{2}\mathbf{x}_{j+1}^T \mathbf{N}\mathbf{x}_{j+1} + \mathbf{x}_{j+1}^T \mathbf{r}$
- (13)         **if**  $f(\mathbf{x}_{j+1}) > \max_{i=0, \dots, \min(j, N_{GLL})} f(\mathbf{x}_{j-i}) + \gamma\lambda \langle \mathbf{d}_j, \mathbf{g}_j \rangle$
- (14)             define  $\lambda_{new} \in [\sigma_{min}\lambda, \sigma_{max}\lambda]$  and repeat line search
- (15)         **else**
- (16)             terminate line search
- (17)          $\mathbf{s}_j = \mathbf{x}_{j+1} - \mathbf{x}_j$
- (18)          $\mathbf{y}_j = \mathbf{g}_{j+1} - \mathbf{g}_j$
- (19)         **if**  $j$  is odd
- (20)              $\hat{\alpha}_{j+1} = \frac{\langle \mathbf{s}_j, \mathbf{P}\mathbf{s}_j \rangle}{\langle \mathbf{s}_j, \mathbf{y}_j \rangle}$
- (21)         **else**
- (22)              $\hat{\alpha}_{j+1} = \frac{\langle \mathbf{s}_j, \mathbf{y}_j \rangle}{\langle \mathbf{y}_j, \mathbf{P}^{-1}\mathbf{y}_j \rangle}$
- (23)          $\hat{\alpha}_{j+1} = \min(\alpha_{max}, \max(\alpha_{min}, \hat{\alpha}_{j+1}))$
- (24)          $w_{j+1} = ||[\mathbf{x}_{j+1} - \Pi_{\mathcal{K}}(\mathbf{x}_{j+1} - \tau_g\mathbf{g}_{j+1})] / \tau_g||_2 = ||\epsilon||_2$
- (25)         **if**  $w_{j+1} \leq \min_{k=0, \dots, j} w_k$
- (26)              $\mathbf{x}_{FB} = \mathbf{x}_{j+1}$
- (27) **return**  $\mathbf{x}_{FB}$

# Kucera Algorithm

ALGORITHM KUCERA( $\mathbf{N}$ ,  $\mathbf{r}$ ,  $\mathbf{x}^0$ ,  $\mathcal{K}$ ,  $\Gamma > 0$ ,  $\tilde{\alpha} \in (0, \|\mathbf{N}\|^{-1}]$ ,  $\epsilon > 0$ )

- (1)  $k = 0$
- (2)  $\mathbf{g} = \mathbf{N}\mathbf{x}^0 + \mathbf{r}$
- (3)  $\mathbf{p} = \phi(\mathbf{x}^0)$
- (4) **while**  $\|\tilde{\mathbf{g}}(\mathbf{x}^k)\| > \epsilon$
- (5)     **if**  $\tilde{\beta}(\mathbf{x}^k)^T \mathbf{g}(\mathbf{x}^k) \leq \Gamma^2 \tilde{\phi}(\mathbf{x}^k)^T \mathbf{g}(\mathbf{x}^k)$
- (6)          $\alpha_{cg} = \mathbf{g}^T \mathbf{p} / \mathbf{p}^T \mathbf{N} \mathbf{p}$
- (7)          $\alpha_f = \min(\alpha_{f,i})$  where  $\alpha_{f,i} = \begin{cases} \mathbf{x}_i / \mathbf{p}_i, & \text{if } \mathbf{p}_i > 0 \\ \infty, & \text{if } \mathbf{p}_i \leq 0 \end{cases}$
- (8)         **if**  $\alpha_{cg} < \alpha_f$
- (9)              $\mathbf{x}^{k+1} = \mathbf{x}^k - \alpha_{cg} \mathbf{p}$
- (10)             $\mathbf{g} = \mathbf{g} - \alpha_{cg} \mathbf{N} \mathbf{p}$
- (11)             $\gamma = \phi(\mathbf{x}^{k+1})^T \mathbf{N} \mathbf{p} / \mathbf{p}^T \mathbf{A} \mathbf{p}$
- (12)             $\mathbf{p} = \phi(\mathbf{x}^{k+1}) - \gamma \mathbf{p}$
- (13)         **else**
- (14)              $\mathbf{x}^{k+1/2} = \mathbf{x}^k - \alpha_f \mathbf{p}$
- (15)              $\mathbf{x}^{k+1} = \mathbf{x}^{k+1/2} - \tilde{\alpha} \tilde{\phi}(\mathbf{x}^{k+1/2})$
- (16)              $\mathbf{g} = \mathbf{N} \mathbf{x}^{k+1} + \mathbf{r}$
- (17)              $\mathbf{p} = \phi(\mathbf{x}^{k+1})$
- (18)         **else**
- (19)              $\mathbf{x}^{k+1} = \mathbf{x}^k - \tilde{\alpha} \tilde{\beta}(\mathbf{x}^k)$
- (20)              $\mathbf{g} = \mathbf{N} \mathbf{x}^{k+1} + \mathbf{r}$
- (21)              $\mathbf{p} = \phi(\mathbf{x}^{k+1})$
- (22)          $k = k + 1$
- (23)     **return**  $\mathbf{x}^k$

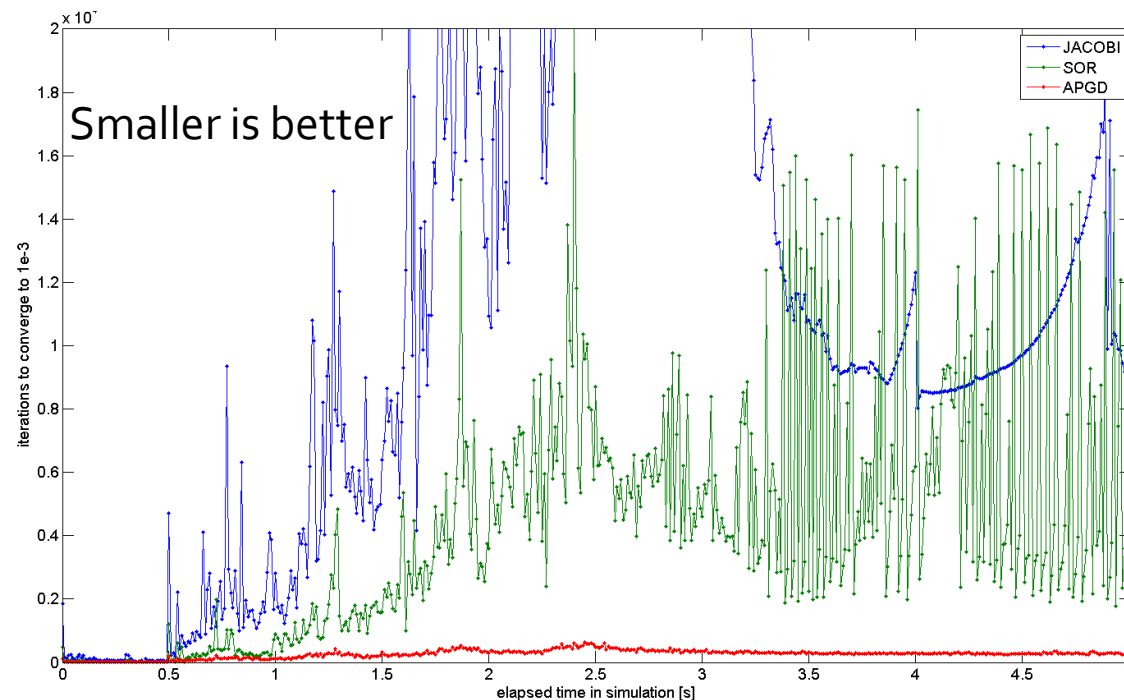
# Nesterov's Accelerated Projected Gradient Descent

ALGORITHM NAPG( $N, r, t \leq \frac{1}{\lambda_{\max}(N)}, \tau, N_{\max}$ )

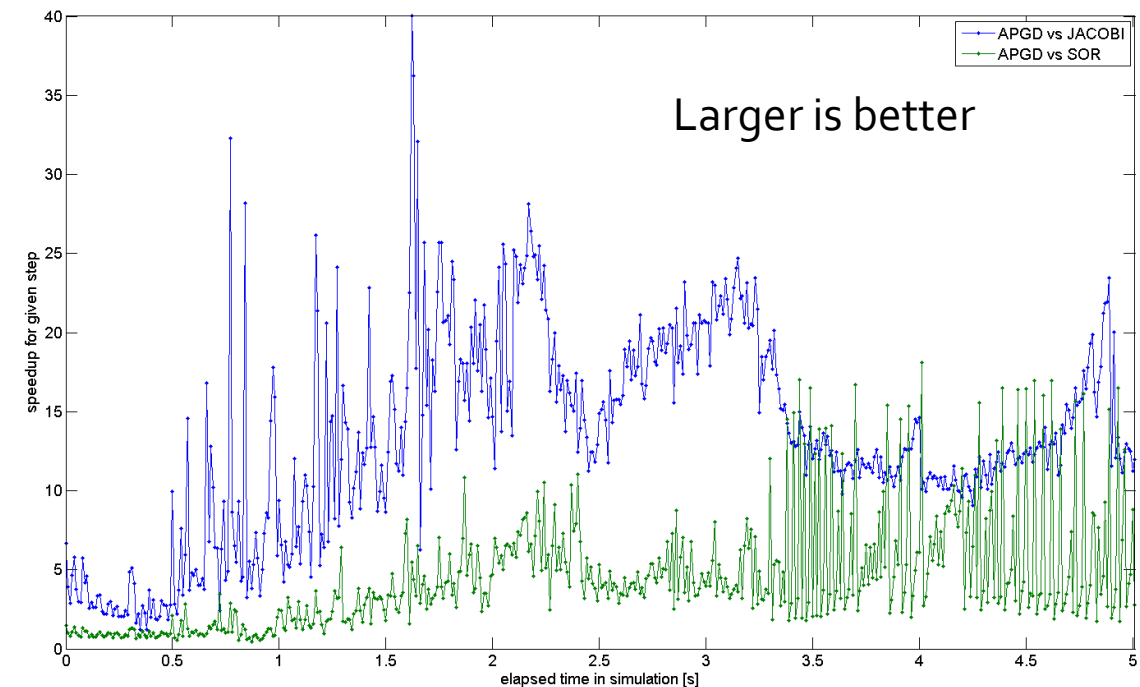
- (1)  $\gamma_0 = \mathbf{0}_{n_c}$
- (2)  $\hat{\gamma}_0 = \mathbf{1}_{n_c}$
- (3)  $\mathbf{y}_0 = \gamma_0$
- (4)  $\theta_0 = 1$
- (5) **for**  $k := 0$  **to**  $N_{\max}$
- (6)      $\mathbf{g} = N\mathbf{y}_k - \mathbf{r}$
- (7)      $\gamma_{k+1} = \Pi_{\mathcal{K}}(\mathbf{y}_k - t\mathbf{g})$
- (8)      $\theta_{k+1} = \frac{-\theta_k^2 + \theta_k \sqrt{\theta_k^2 + 4}}{2}$
- (9)      $\beta_{k+1} = \theta_k \frac{1 - \theta_k}{\theta_k^2 + \theta_{k+1}}$
- (10)     $\mathbf{y}_{k+1} = \gamma_{k+1} + \beta_{k+1}(\gamma_{k+1} - \gamma_k)$
- (11)     $\epsilon = \epsilon(\gamma_{k+1})$
- (12)    **if**  $\epsilon < \tau$
- (13)        **break**
- (14)    **endif**
- (15) **endfor**
- (16) **return** Value at time step  $t_{l+1}, \gamma^{l+1} := \hat{\gamma}$ .

# Relative Speedup: Benchmark Problem [1000 bodies]

## Number of iterations to convergence

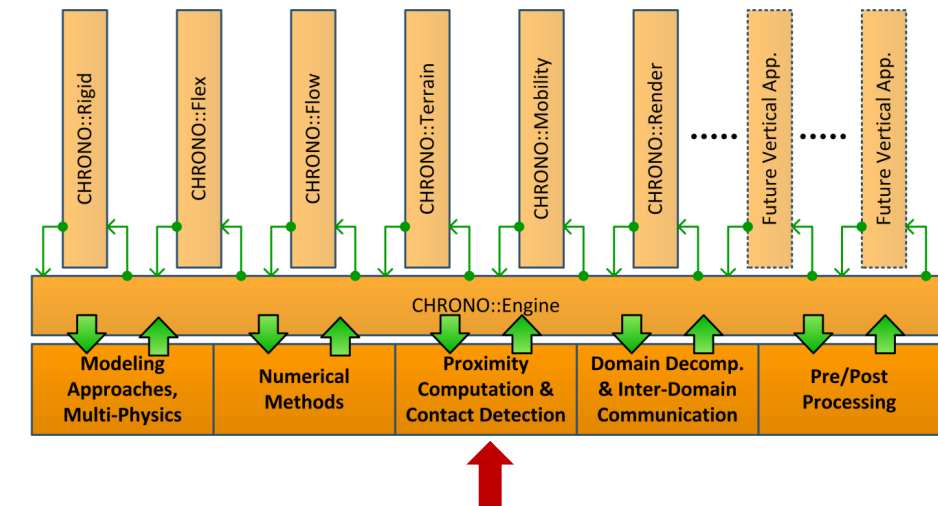


## Speedup: APGD vs. Jacobi and SOR

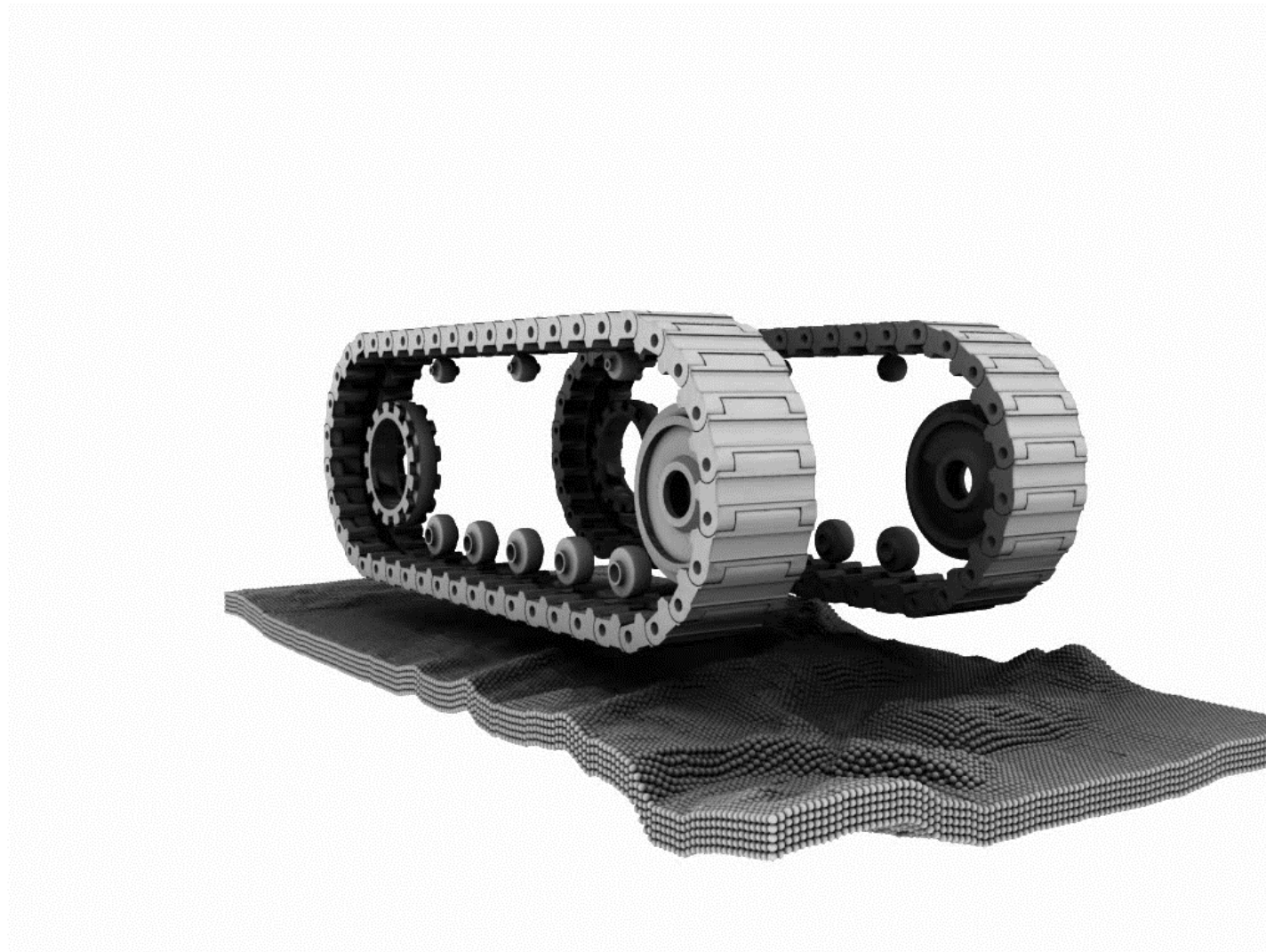


# Proximity computation

- Advanced modeling techniques
- Algorithmic (applied math) support
- Proximity computation
- Domain decomposition & Inter-domain data exchange
- Post-processing (visualization)



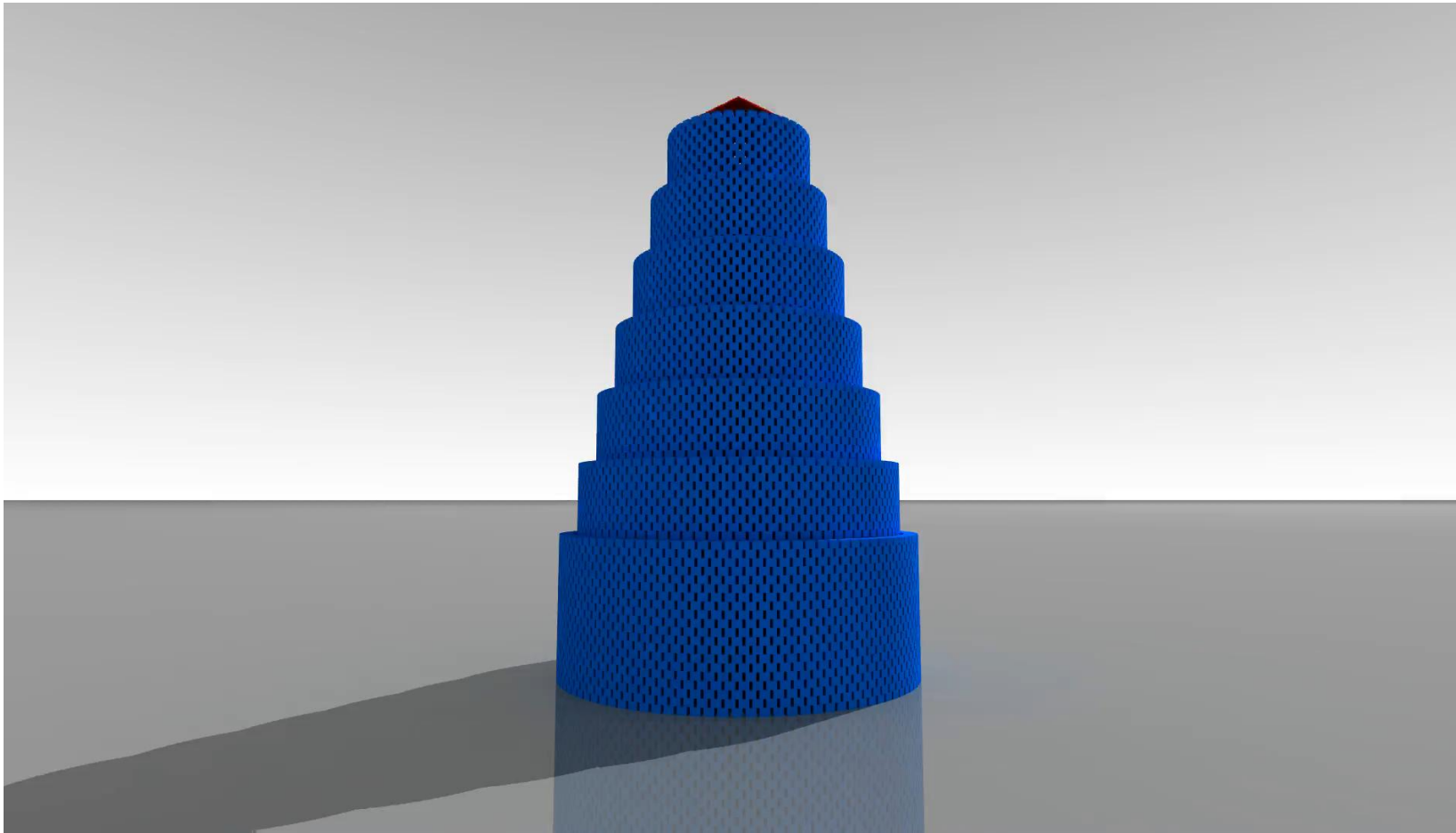
# Tracked Vehicle Simulation





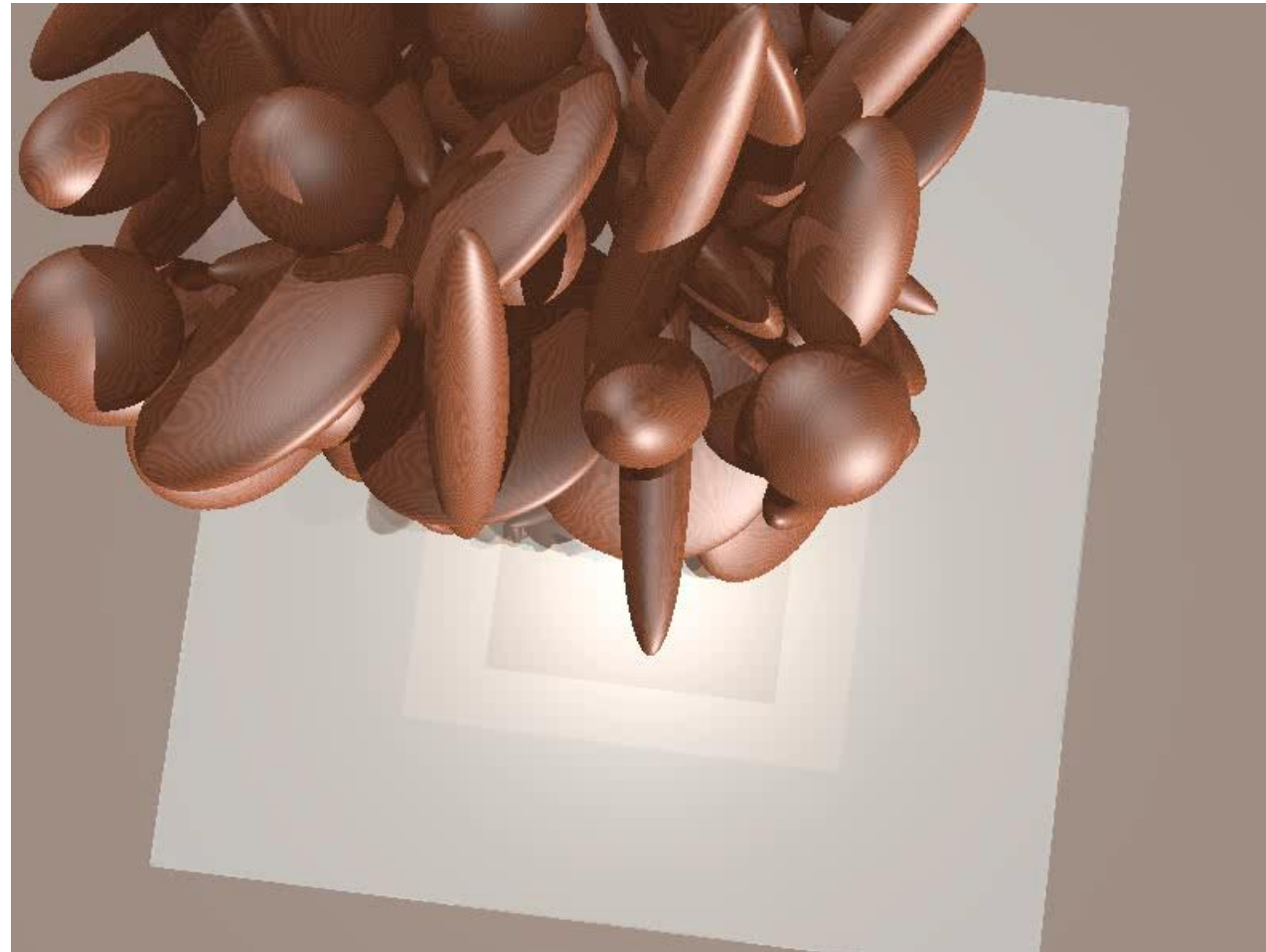
# 600,000 Bodies Moving & Colliding

[run on the GPU]





# Ellipsoid-Ellipsoid CD



# Various Geometries Handled...

## [Ellipsoid-Ellipsoid Example]

$$\mathbf{d} = \mathbf{P}_1 - \mathbf{P}_2 = \left( \frac{1}{2\lambda_1} \mathbf{M}_1 + \frac{1}{2\lambda_2} \mathbf{M}_2 \right) \mathbf{c} + (\mathbf{b}_1 - \mathbf{b}_2)$$

$$\frac{\partial \mathbf{d}}{\partial \alpha_i} = \frac{\partial \mathbf{P}_1}{\partial \alpha_i} - \frac{\partial \mathbf{P}_2}{\partial \alpha_i}, \quad \frac{\partial^2 \mathbf{d}}{\partial \alpha_i \partial \alpha_j} = \frac{\partial^2 \mathbf{P}_1}{\partial \alpha_i \partial \alpha_j} - \frac{\partial^2 \mathbf{P}_2}{\partial \alpha_i \partial \alpha_j}$$

$$\frac{\partial \mathbf{P}}{\partial \alpha_i} = \left( \frac{1}{2\lambda} \mathbf{M} - \frac{1}{8\lambda^3} \mathbf{M} \mathbf{c} \mathbf{c}^T \mathbf{M} \right) \frac{\partial \mathbf{c}}{\partial \alpha_i}$$

$$\begin{aligned} \frac{\partial^2 \mathbf{P}}{\partial \alpha_i \partial \alpha_j} = & \left( -\frac{1}{8\lambda^3} \mathbf{M} + \frac{3}{32\lambda^5} \mathbf{M} \mathbf{c} \mathbf{c}^T \mathbf{M} \right) \mathbf{c}^T \mathbf{M} \frac{\partial \mathbf{c}}{\partial \alpha_j} \frac{\partial \mathbf{c}}{\partial \alpha_i} \\ & - \frac{1}{8\lambda^3} \left[ \left( \mathbf{c}^T \mathbf{M} \frac{\partial \mathbf{c}}{\partial \alpha_i} \right) \mathbf{M} + \mathbf{M} \mathbf{c} \left( \frac{\partial \mathbf{c}}{\partial \alpha_i} \right)^T \mathbf{M} \right] \frac{\partial \mathbf{c}}{\partial \alpha_j} \\ & + \left( \frac{1}{2\lambda} \mathbf{M} - \frac{1}{8\lambda^3} \mathbf{M} \mathbf{c} \mathbf{c}^T \mathbf{M} \right) \frac{\partial^2 \mathbf{c}}{\partial \alpha_i \partial \alpha_j} \end{aligned}$$

$$\varepsilon: \frac{x^2}{r_1^2} + \frac{y^2}{r_2^2} + \frac{z^2}{r_3^2} = 1$$

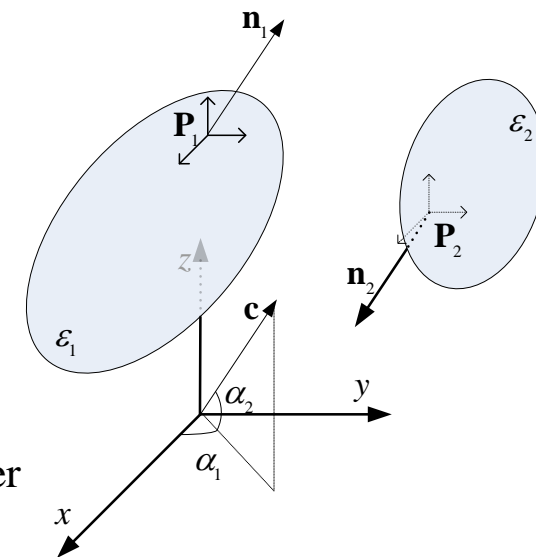
$\mathbf{A}$  : Rotation Matrix

$$\mathbf{M} = \mathbf{A} \mathbf{R}^2 \mathbf{A}^T$$

$$\mathbf{R} = \text{diag}(r_1, r_2, r_3)$$

$\mathbf{b}$  : Translation of  
ellipsoids center

$$\lambda^2 = \frac{1}{4} \mathbf{n}^T \mathbf{M} \mathbf{n}$$



$$\mathbf{d} = \mathbf{P}_1 - \mathbf{P}_2$$

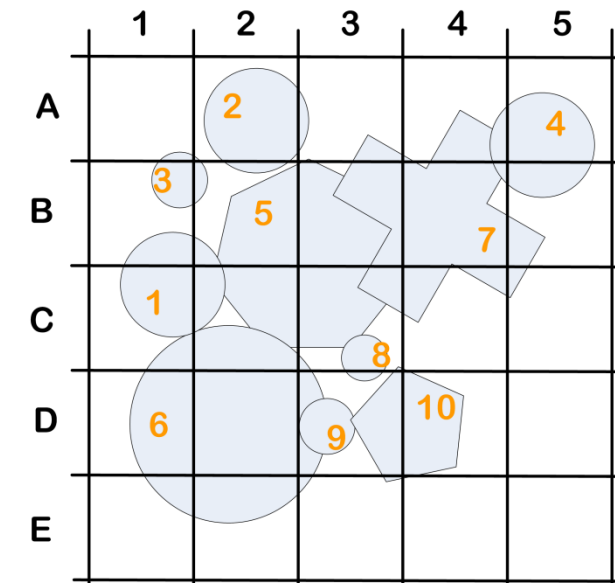
$$\min_{\alpha_1, \alpha_2} \|d(\alpha_1, \alpha_2)\|^2$$

# Collision Detection

- Broad phase
  - Draws on an Axis Aligned Bounding Box (AABB) approach
- Narrow phase
  - Draws on Minkowski Portal Refinement

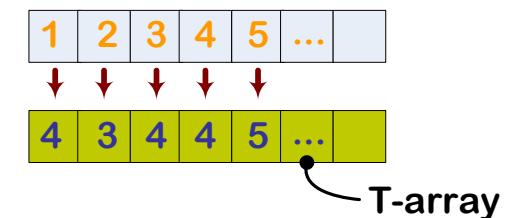
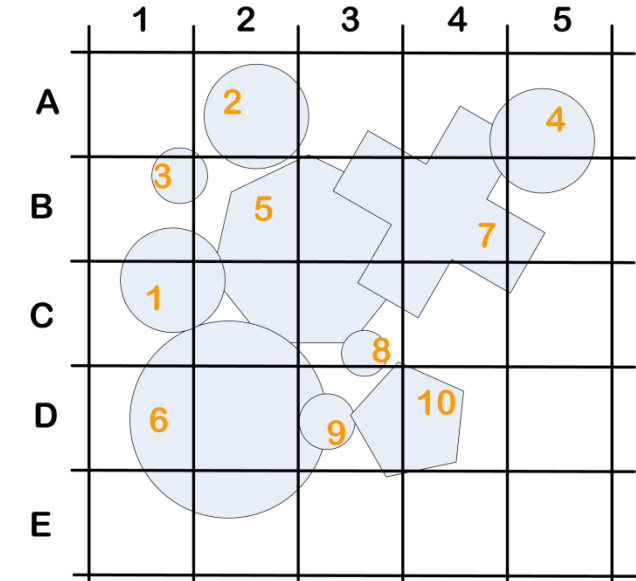
# CD: Binning

- Example: 2D collision detection, bins are squares
- Body 4 touches bins A<sub>4</sub>, A<sub>5</sub>, B<sub>4</sub>, B<sub>5</sub>
- Body 7 touches bins A<sub>3</sub>, A<sub>4</sub>, A<sub>5</sub>, B<sub>3</sub>, B<sub>4</sub>, B<sub>5</sub>, C<sub>3</sub>, C<sub>4</sub>, C<sub>5</sub>
- In proposed algorithm, bodies 4 and 7 will be checked for collision by three threads (associated with bin A<sub>4</sub>, A<sub>5</sub>, B<sub>4</sub>)



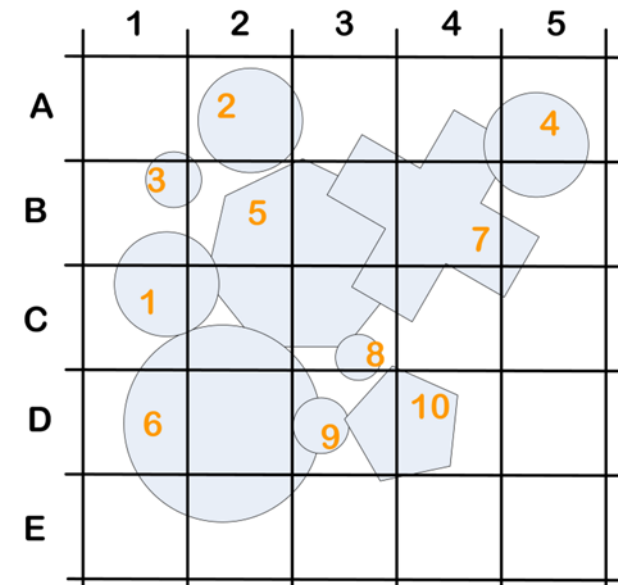
# Stage 1 (Body Parallel)

- Purpose: find the number of bins touched by each body
- Store results in the “T”, array of N integers
- Key observation: it’s easy to bin bodies



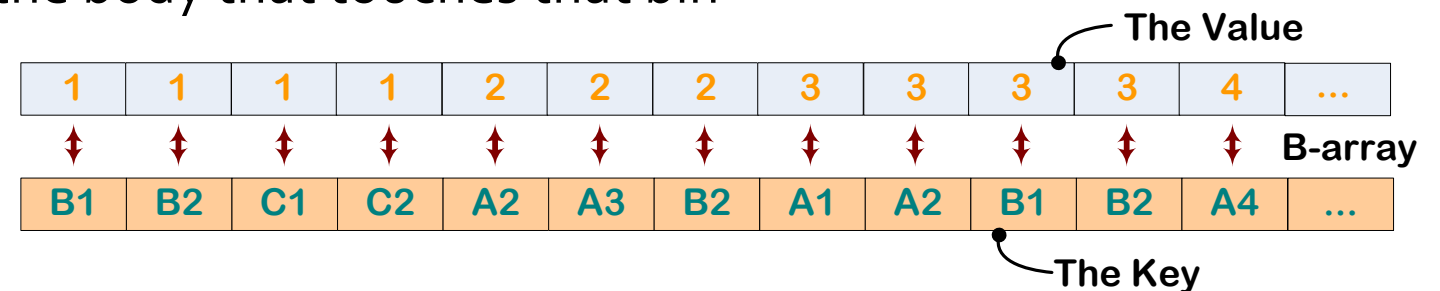
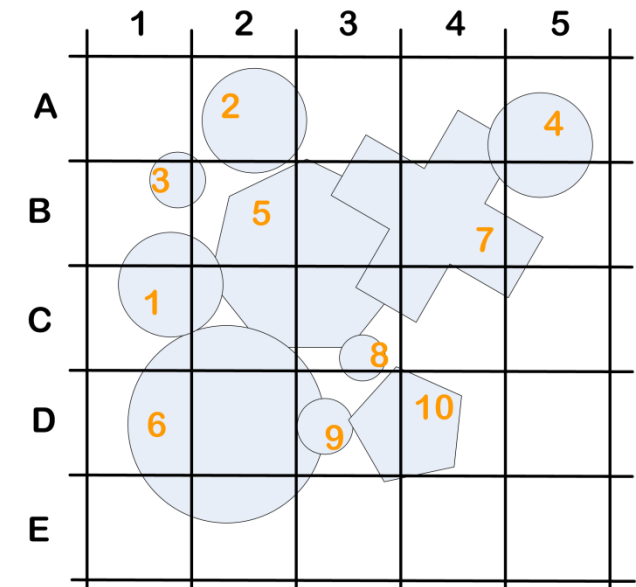
## Stage 2: Parallel Inclusive Scan

- Run a parallel inclusive scan on the array **T**
  - The last element is the total number of bin touches, including the last body
- Complexity of Stage:  $O(N)$  – using **thrust** library
- Purpose: determine the number of entries **M** needed to store the indices of all the bins touched by each body in the problem



## Stage 3: Determine bin-to-body association

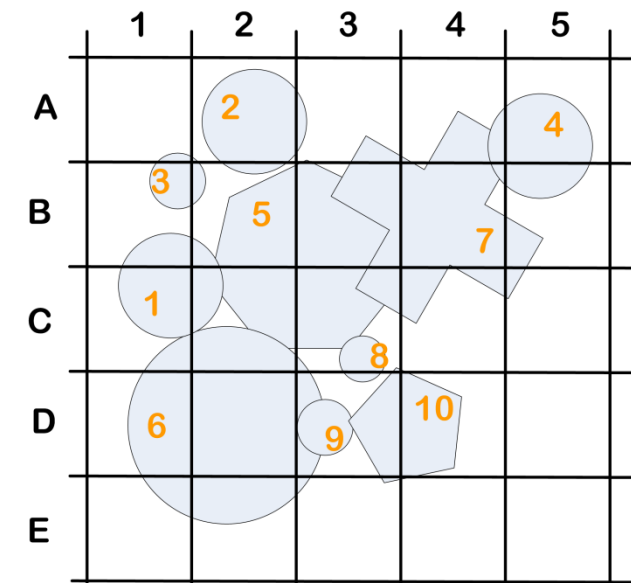
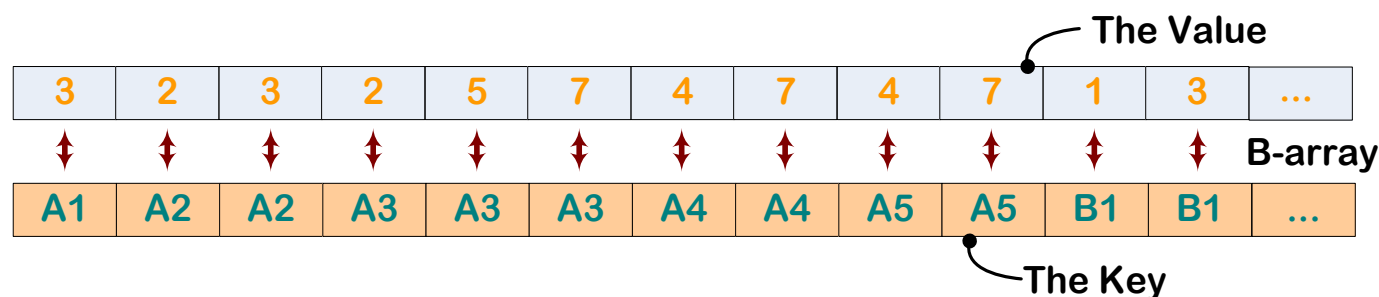
- Stage executed in parallel on a per-body basis
- Allocate an array **B** of M pairs of integers.
- The key (first entry of the pair), is the bin index
- The value (second entry of pair) is the body that touches that bin





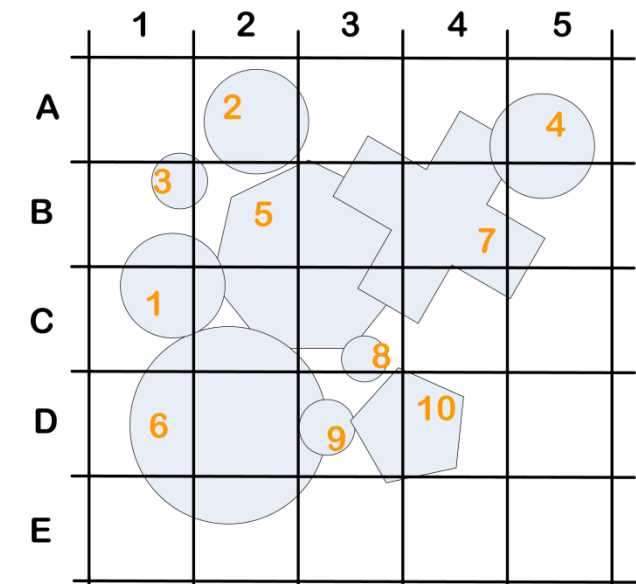
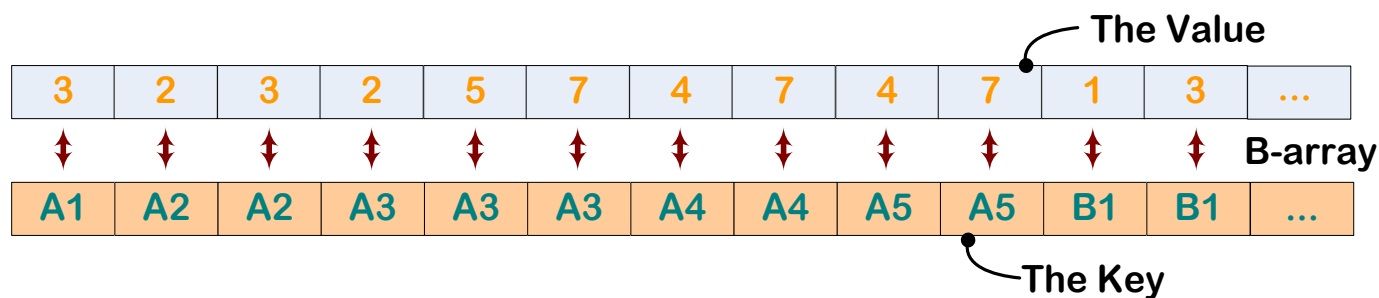
## Stage 4: Radix Sort

- In parallel, run radix sort to order the **B** array according to key values
- Work load:  $O(N)$
- Relies on **thrust** library



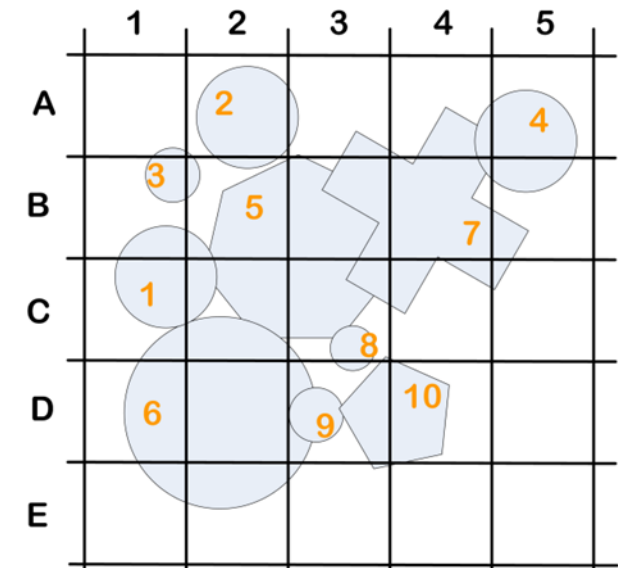
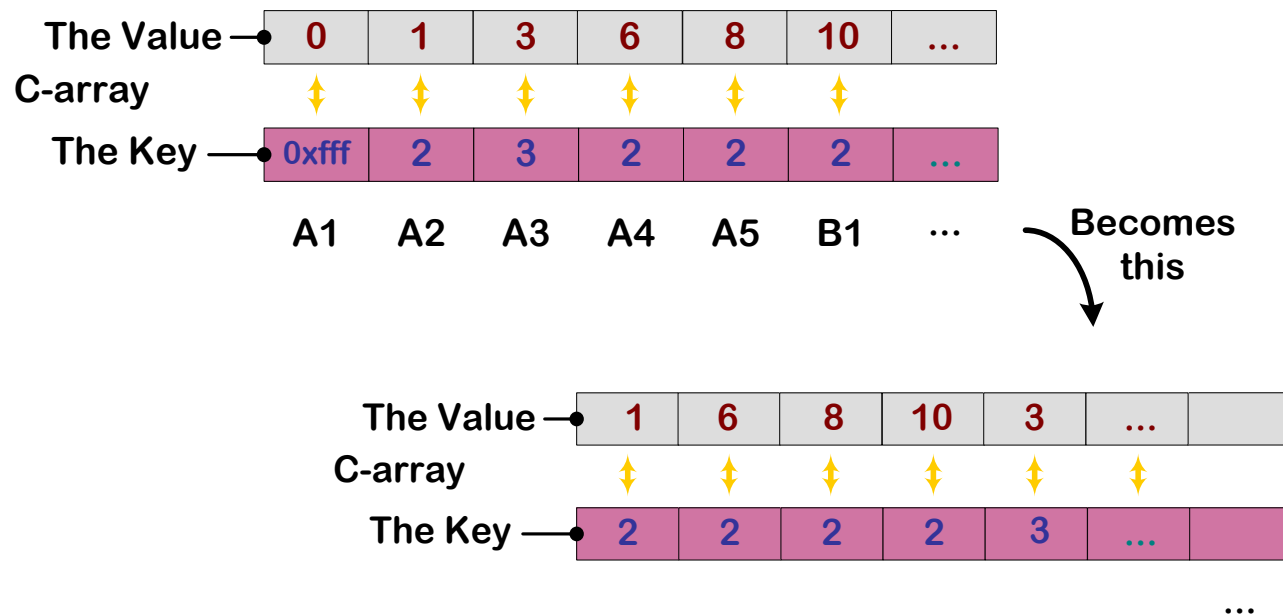
## Stage 5: Find Bin Starting Index

- Host allocates on device an array of length  $N_b$  of pairs of unsigned integers
- Run in parallel, on a per bin basis:
  - Load in parallel in shared memory chunks of the **B** array and find the location where each bin starts
  - Store it in entry  $k$  of **C**, as the key associated with this pair
  - Key of bins with one or no bodies is set to maximum unsigned int value of 0xffffffff



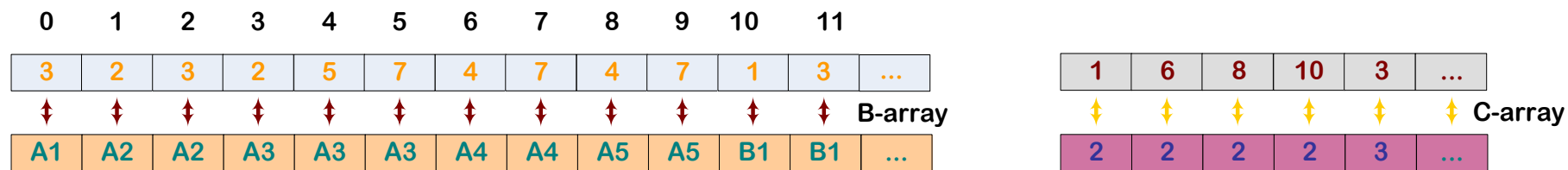
## Stage 6: Sort **C** for Pruning

- Do a parallel radix sort on the array **C** based on the key
- Purpose: move unused bins to the end of array
- Effort:  $O(N_b)$



# Stage 7: Investigate Collisions in each Bin

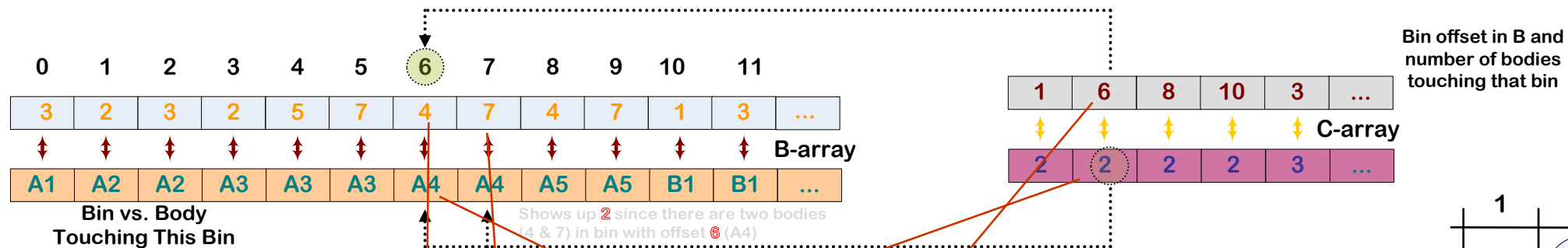
- Carried out in parallel, one thread per bin



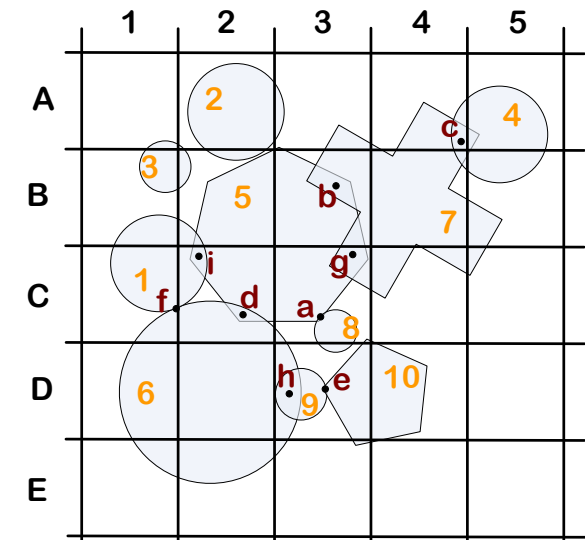
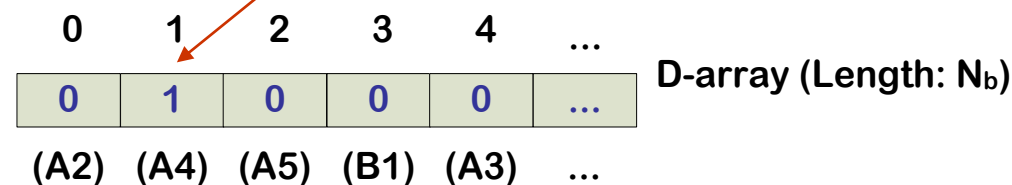
- To store information generated during this stage host allocates unsigned integer array **D** of length  $N_b$ 
  - Array **D** stores the number of actual contacts occurring in each bin
  - D** is in sync with (linked to) **C**, which in turn is in sync with (linked to) **B**
- Parallelism: one thread per bin
  - Thread  $k$  reads the pair key-value in entry  $k$  of array **C**
  - Thread  $k$  reads does rehearsal for brute force collision detection
  - Outcome: the number  $s$  of active collisions taking place in a bin
  - Value  $s$  stored in  $k^{\text{th}}$  entry of the **D** array

# Stage 7: Details...

- Recall that how C is organized is a reflection of how B is organized

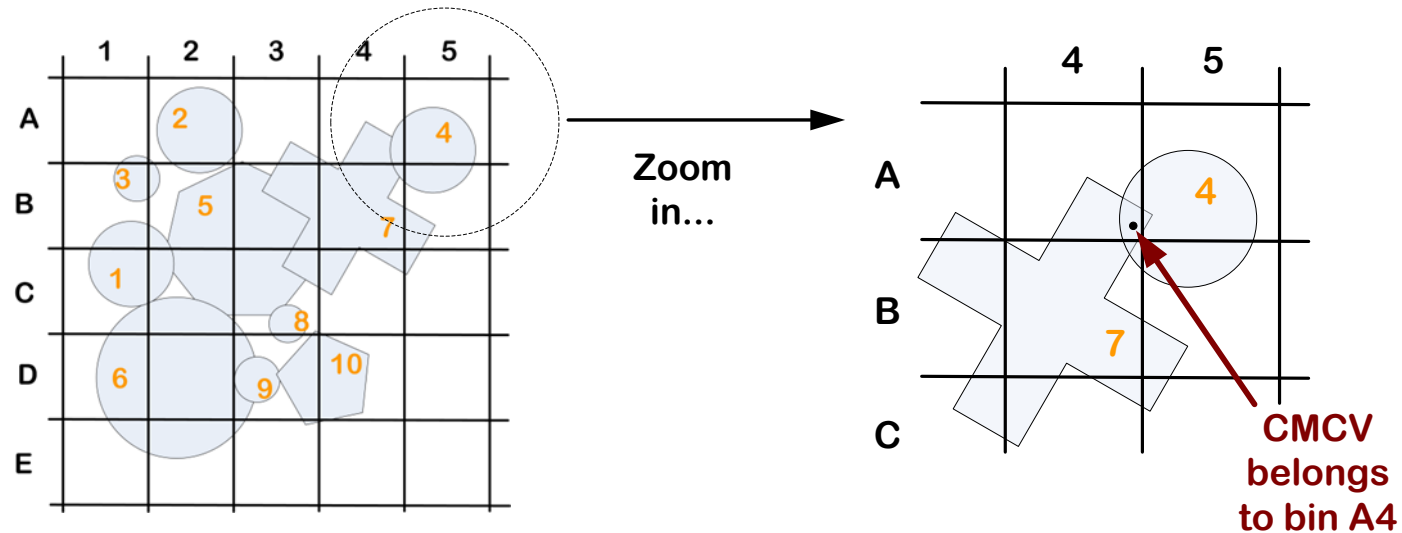


- The drill: thread 0 relies on info at  $C[0]$ , thread 1 relies on info at  $C[1]$ , etc.
- Let's see what thread 2 (goes with  $C[2]$ ) does:
  - Read the first 2 bodies that start at offset 6 in B.
    - These bodies are 4 and 7, and as B indicates, they touch bin A4
    - Bodies 4 and 7 turn out to have 1 contact in A4, which means that entry 2 of D needs to reflect this



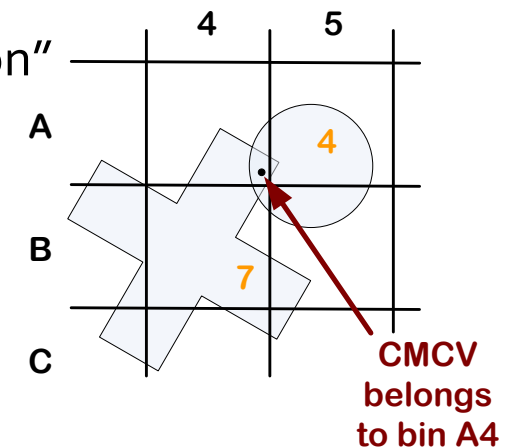
# Stage 7: Details...

- Brute Force CD rehearsal
- Carried out to understand the memory requirements associated with collisions in each bin
- Finds out the total number of contacts owned by a bin
- Key question: which bin does a contact belong to?
- Answer: It belongs to bin containing the CM of the Contact Volume (CMCV)



## Stage 7, Comments

- Two bodies can have multiple contacts, handled ok by the method
- Easy to define the CMCV for two spheres, two ellipsoids, and a couple of other simple geometries
  - In general finding CMCV might be tricky
    - Notice picture below, CM of 4 is in A<sub>5</sub>, CM of 7 is in B<sub>4</sub> and CMCV is in A<sub>4</sub>
- Finding the CMCV is the subject of the so called “narrow phase collision detection”
  - It’ll be simple in our case since we are going to work with simple geometry primitives





# Stage 8: Inclusive Prefix Scan

- Save to the side the number of contacts in the last bin (last entry of **D**)  $d_{last}$ 
  - Last entry of **D** will get overwritten

0	1	2	3	4	...
0	1	0	0	0	...
(A2)	(A4)	(A5)	(B1)	(A3)	...

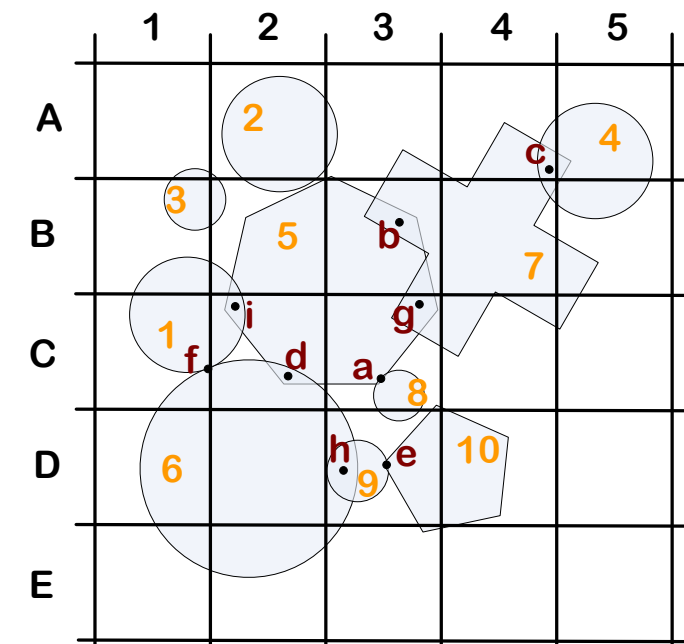
**D-array (Length:  $N_b$ )**

- Run parallel exclusive prefix scan on **D**:

0	1	2	3	4	...
0	0	1	1	1	...
(A2)	(A4)	(A5)	(B1)	(A3)	...

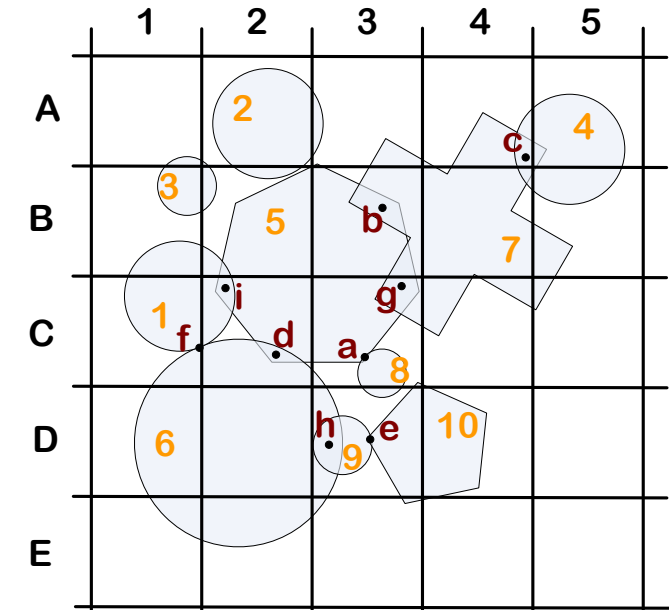
**D-array, after exclusive prefix scan**

- Total number of actual collisions:  $N_c = \mathbf{D}[N_b] + d_{last}$



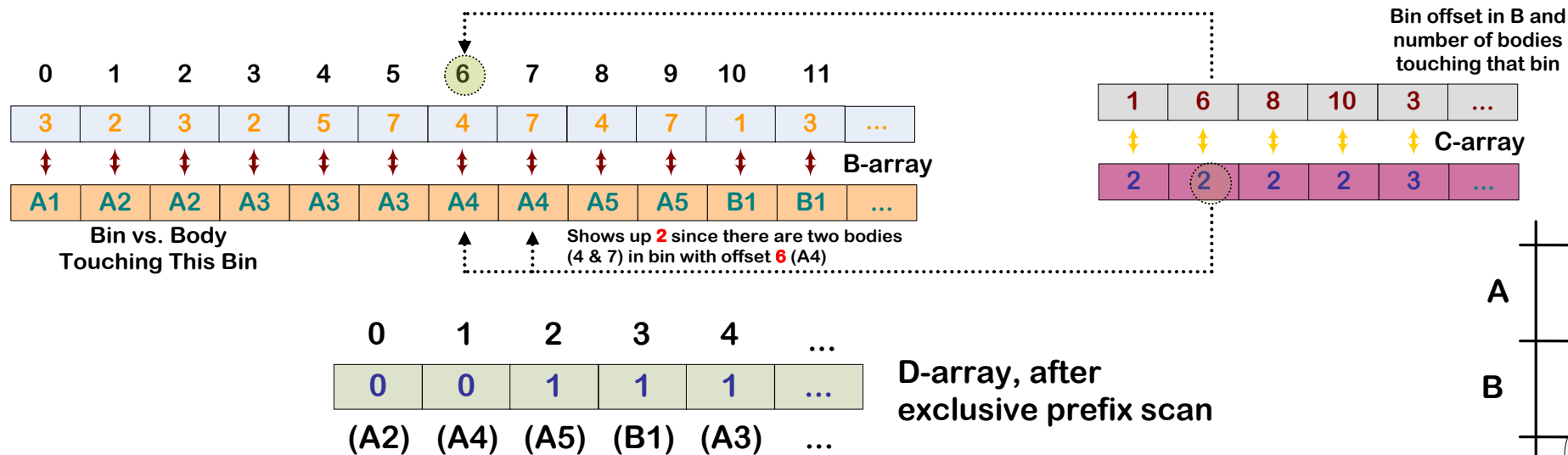
## Stage 9: Populate Array E

- From the host, allocate on the device memory for array **E**
  - Array **E** stores the required collision information: normal, two tangents, etc.
  - Number of entries in the array:  $N_c$  (see previous slide)
- In parallel, on a per bin basis (one thread/bin):
  - Populate the **E** array with required info
- Not discussed in greater detail, this is just like Stage 7, but now you have to generate actual collision info (stage 7 was the rehearsal)
- Thread for  $A_4$  will generate the info for contact "c"
- Thread for  $C_2$  will generate the info for "i" and "d"
- Etc.



# Stage 9, details

- **B**, **C**, **D** required to populate array **E** with collision information



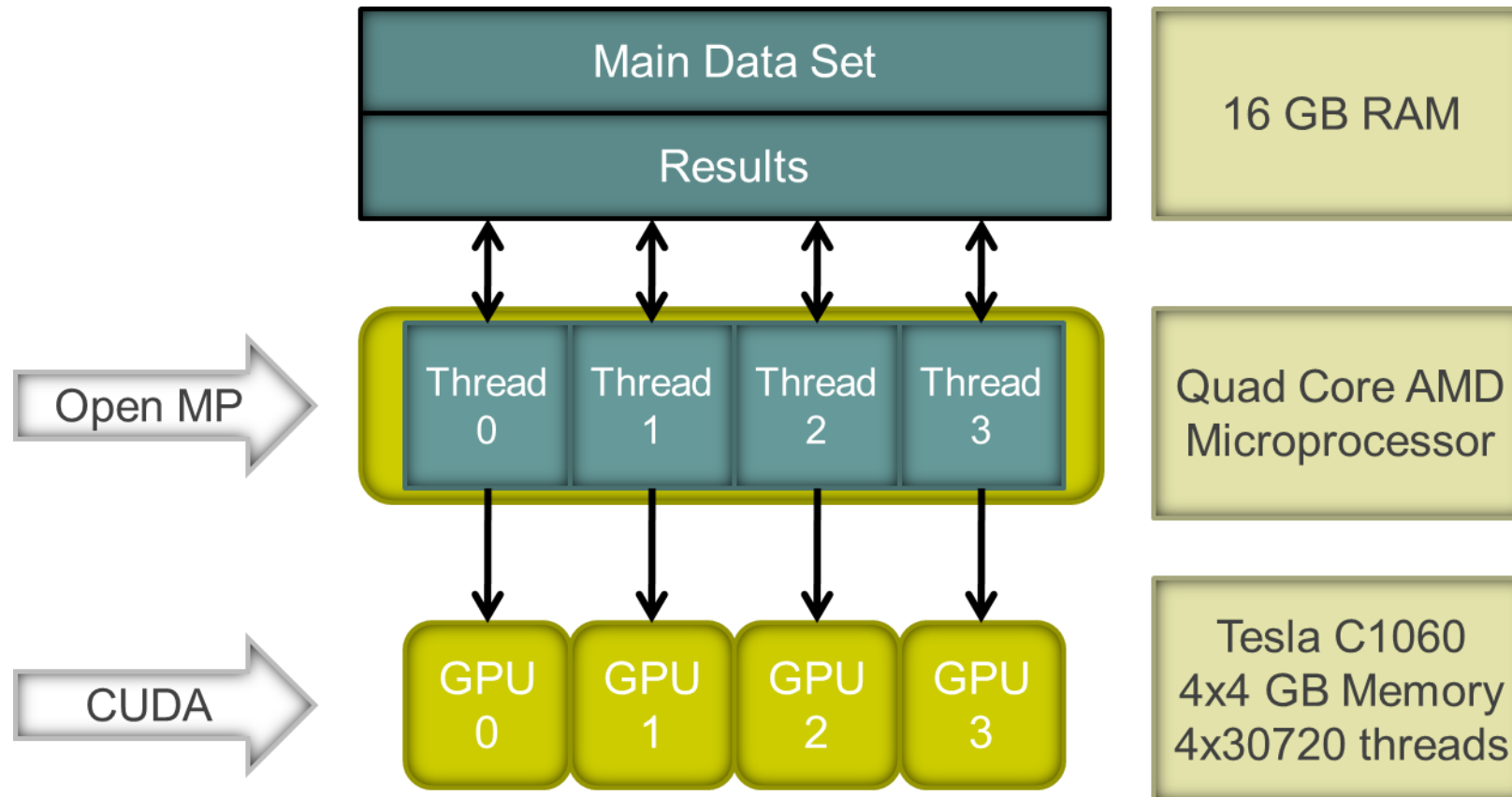
- **C** and **B** are needed to compute the collision information
- **D** needed to understand where collision information is stored in **E**

# Multiple-GPU Collision Detection

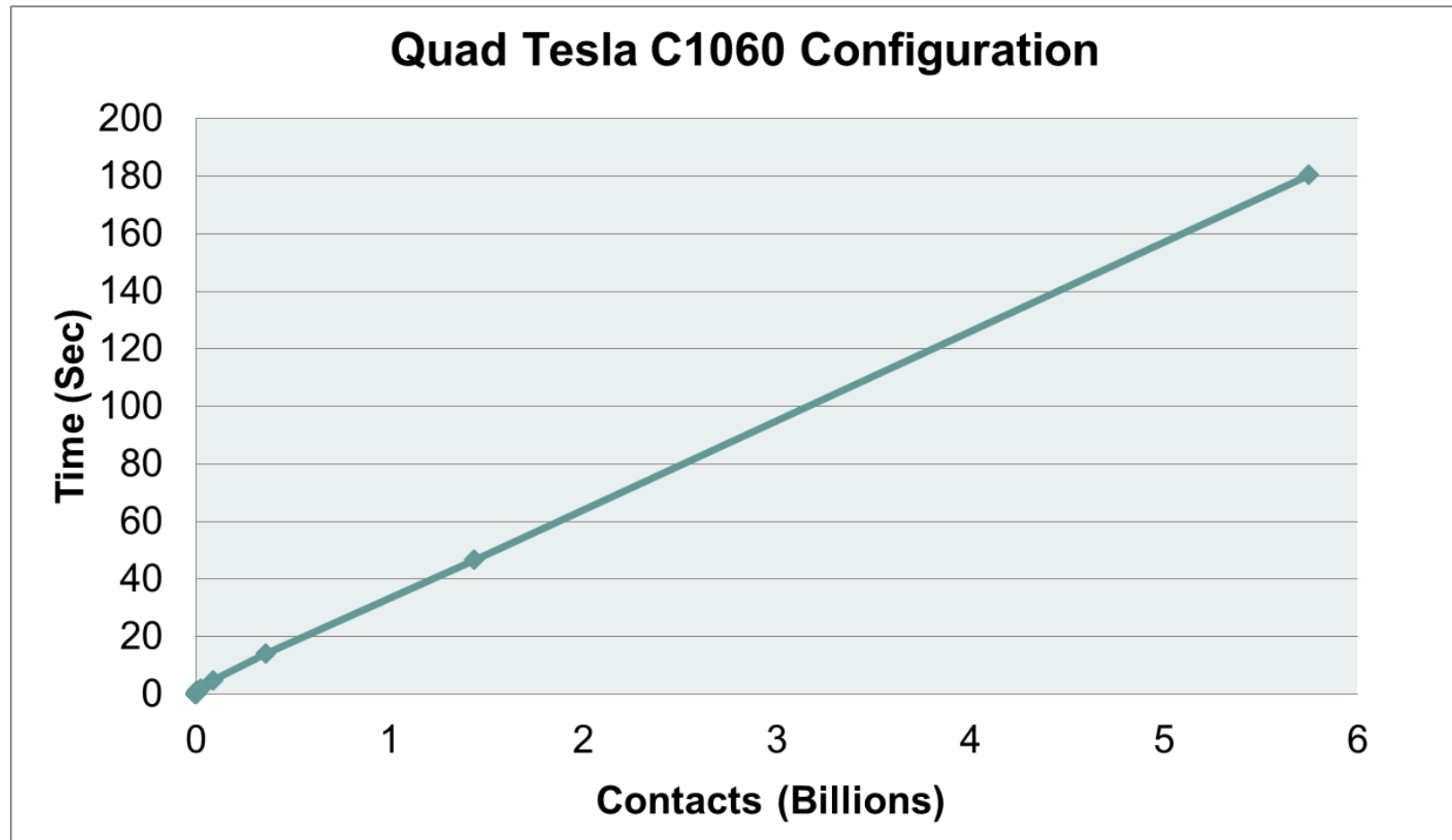
- Processor: AMD Phenom II X4 940 Black
- Memory: 16GB DDR2
- Graphics: 4x NVIDIA Tesla C1060
- Power supply 1: 1000W
- Power supply 2: 750W



# Software/Hardware Setup

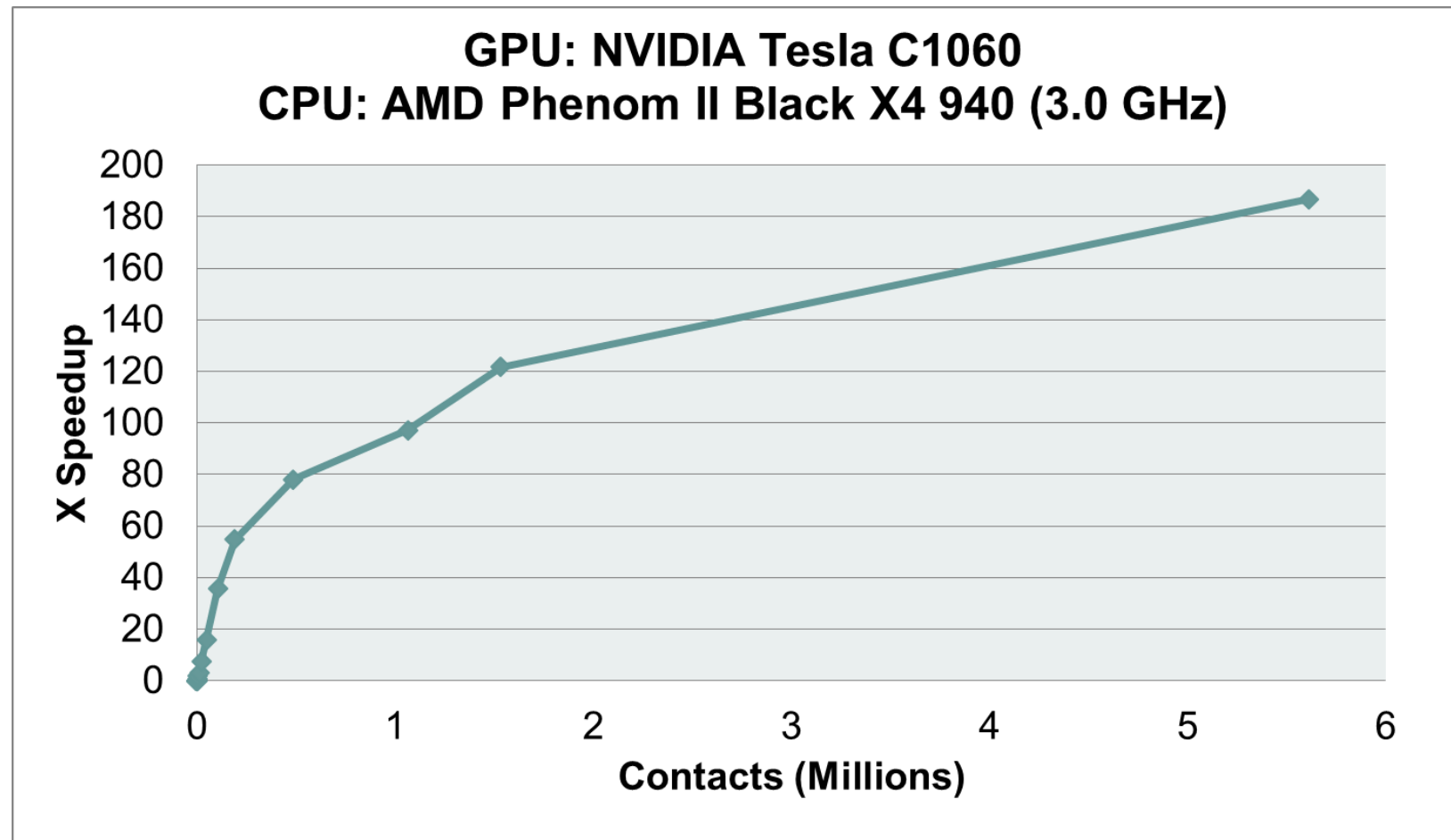


# Spheres – Contacts vs. Time



# Speedup - GPU vs. CPU (Bullet library)

[results reported are for spheres]





# Domain decomposition & Inter-domain data exchange

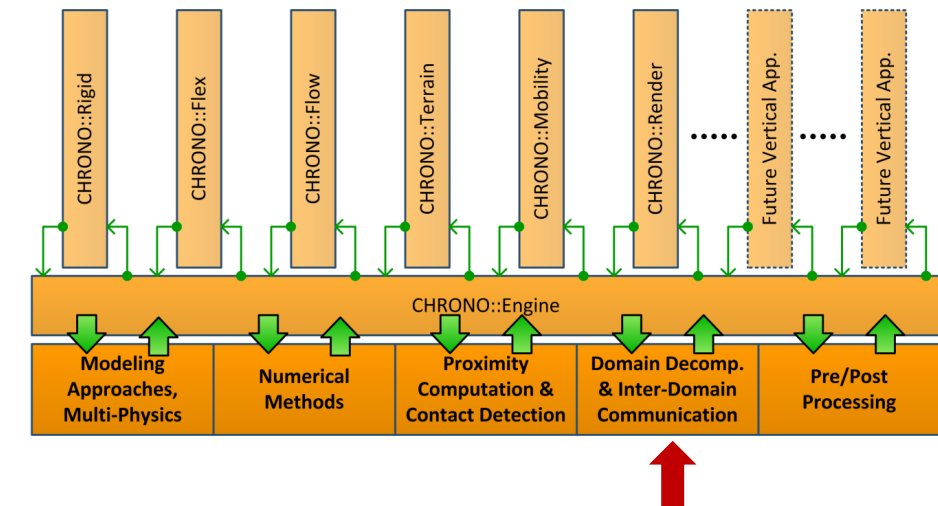
Advanced modeling techniques

Algorithmic (applied math) support

Proximity computation

Domain decomposition & Inter-domain data exchange

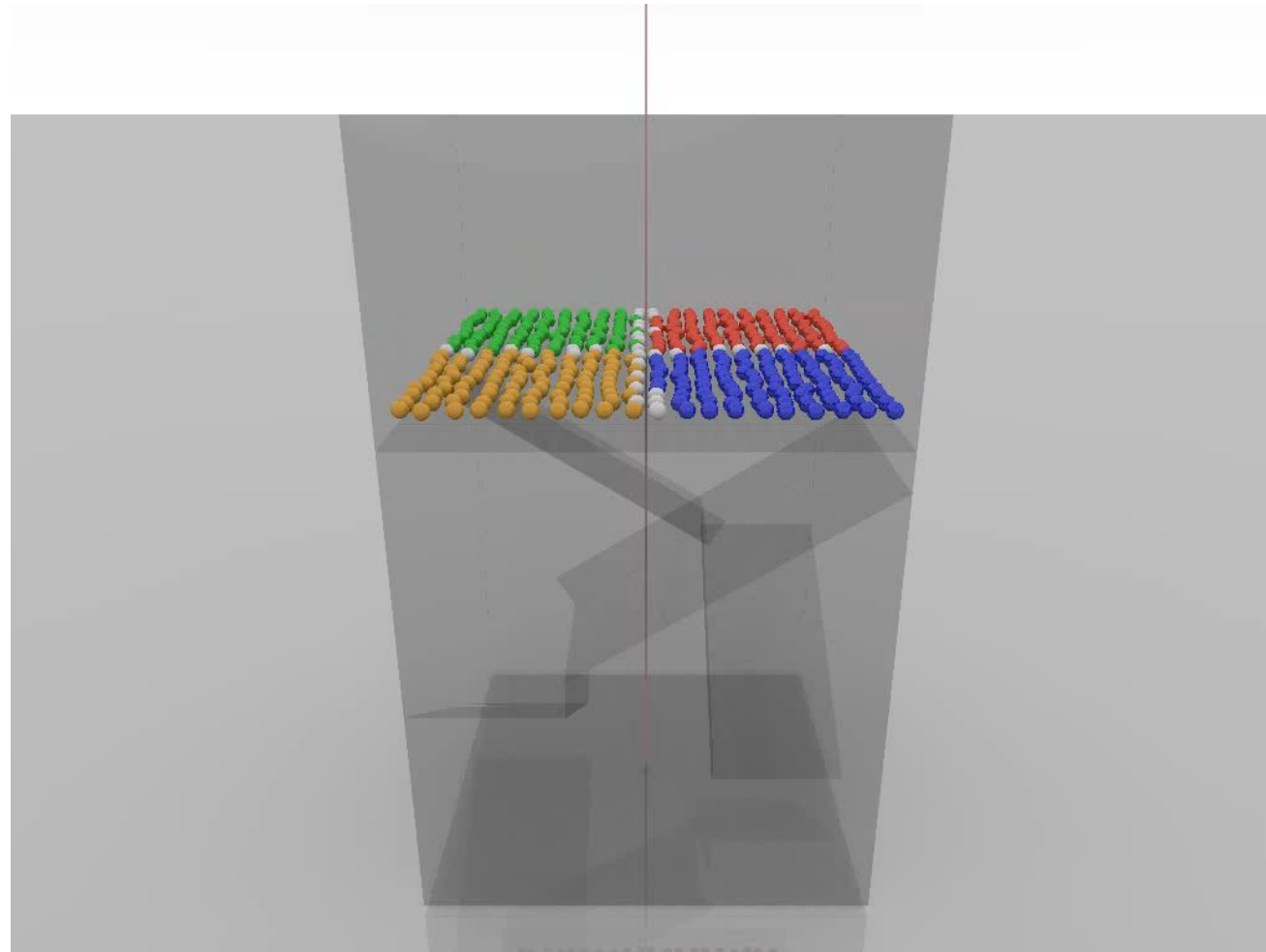
Post-processing (visualization)



# Juggling World Record: 64 People Juggling (of all places) in Madison, Wisconsin



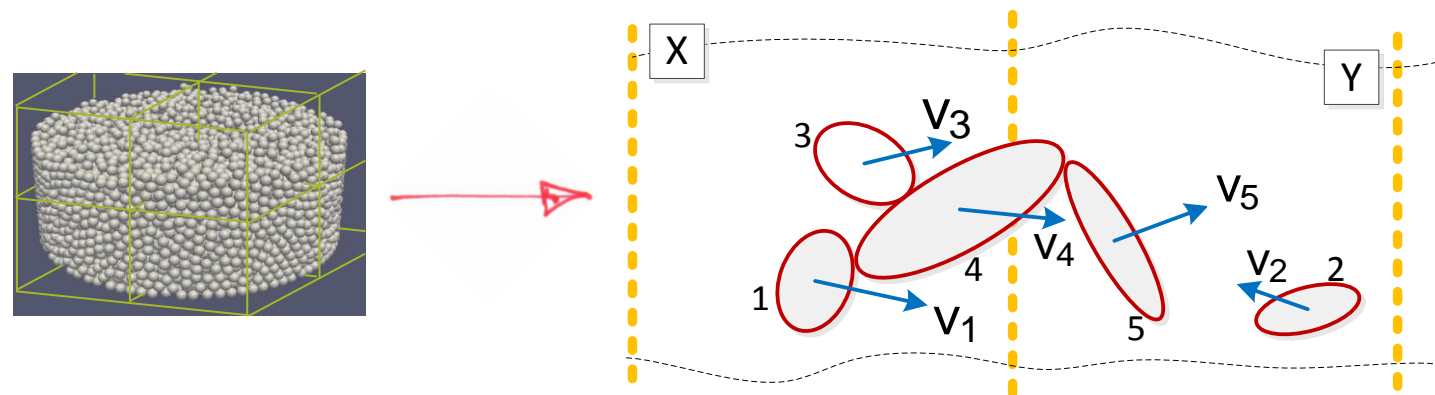
# Computation Using Multiple CPUs



# CHRONO:

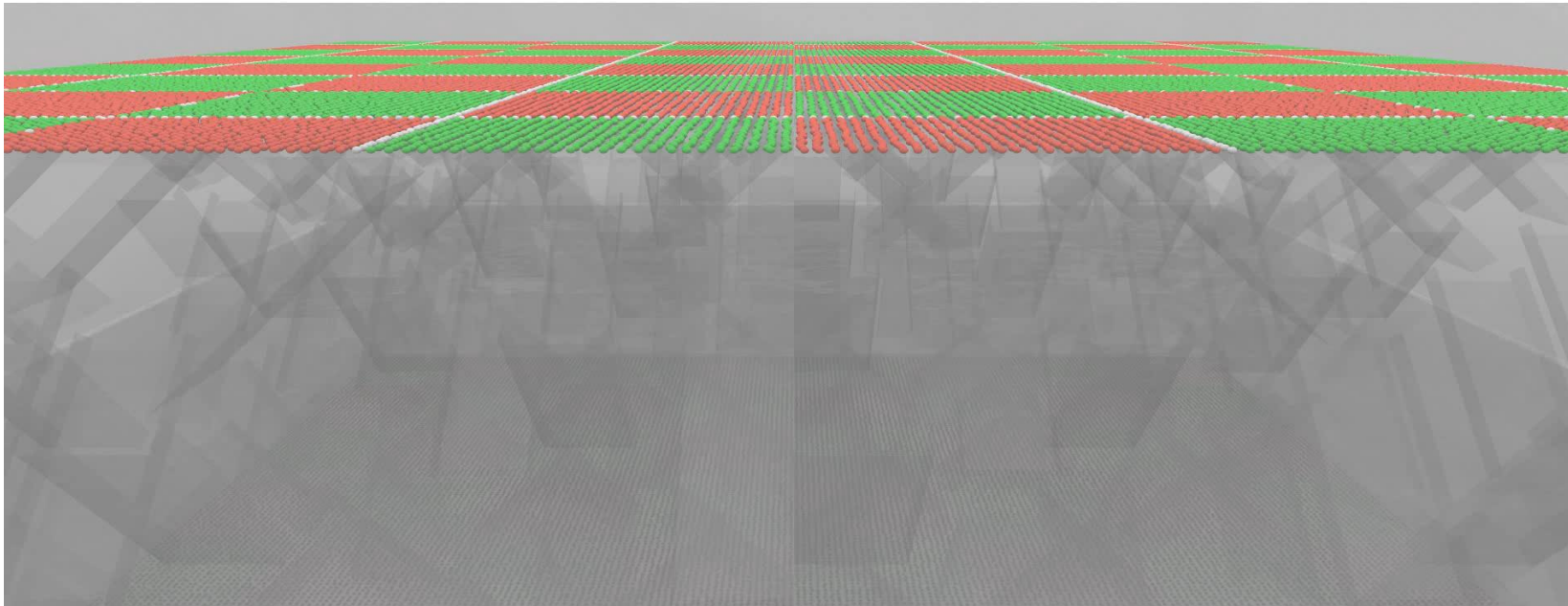
## Domain decomposition & Inter-domain data exchange

- Divide simulation into chunks and have multiple CPUs/GPUs exchange data during simulation, as needed
- Elements leave one subdomain to move to a different one in transparent fashion
- Key issues:
  - Dynamic load balancing
  - Establish a dynamic data exchange protocol (DDEP) between sub-domains

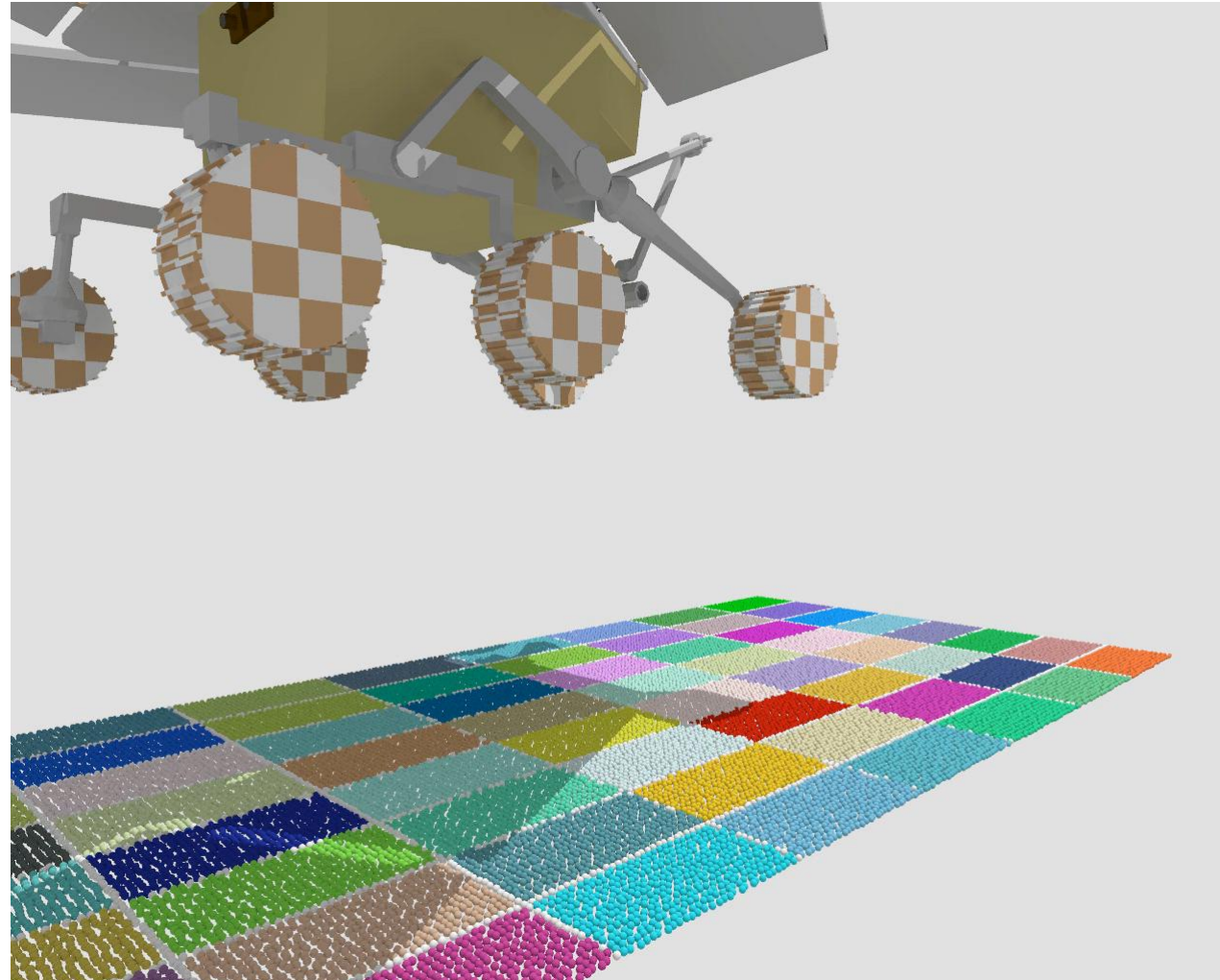


# 0.5 Million Bodies on 64 Cores

[Penalty Approach, MPI-based]



# Computation Using Multiple CPUs





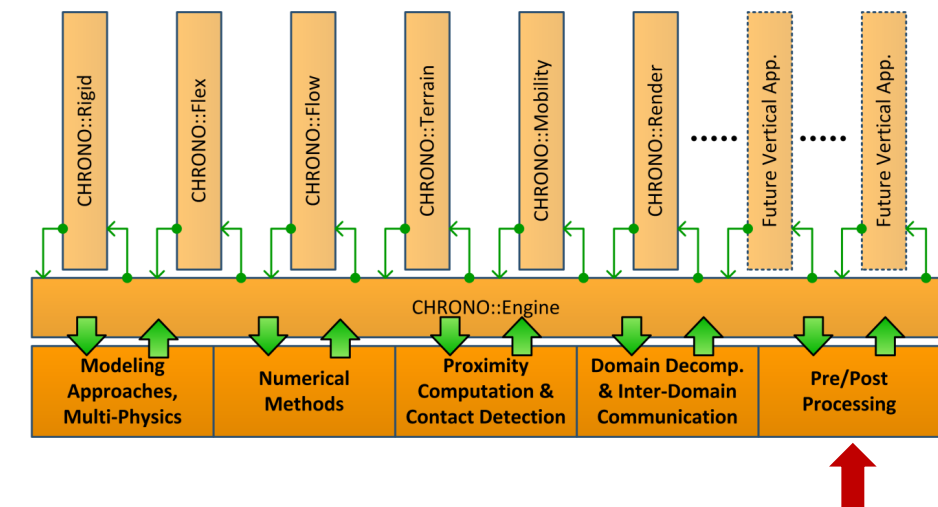
# Rover Footprint, Multi-Domain Computation





# Pre/Post-processing (visualization)

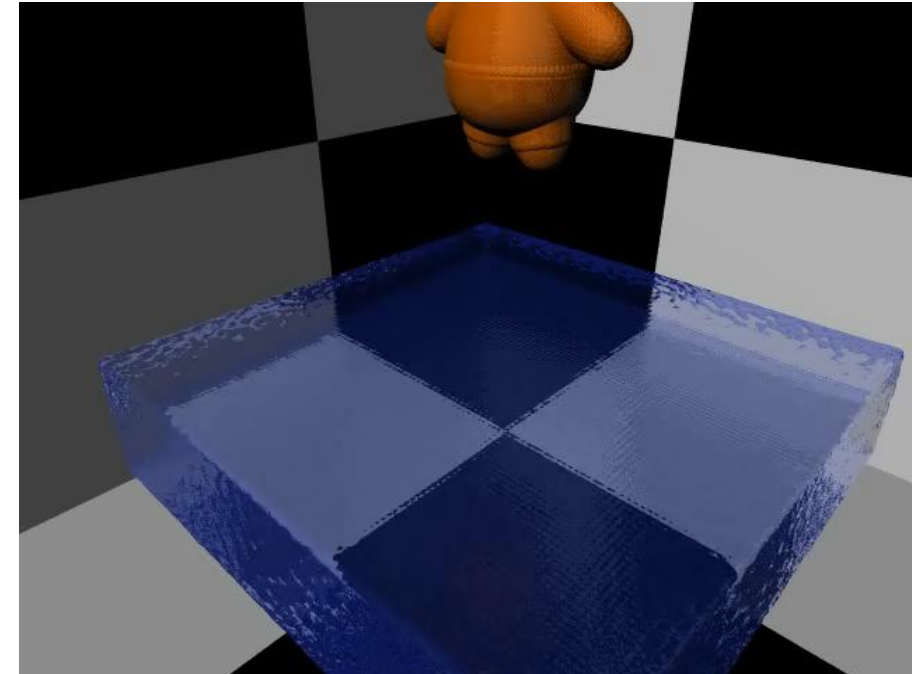
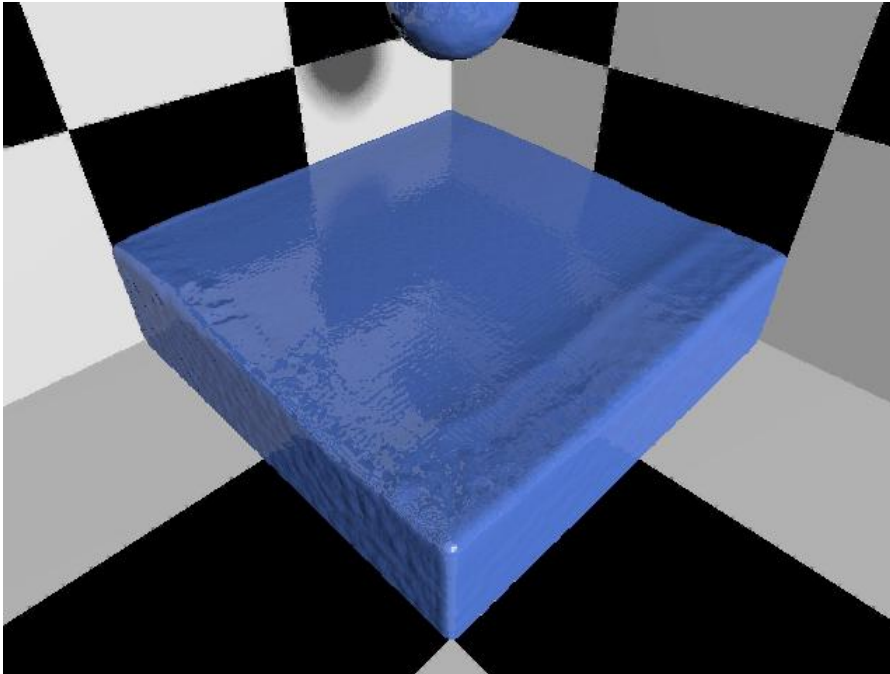
- Advanced modeling techniques
- Algorithmic (applied math) support
- Proximity computation
- Domain decomposition & Inter-domain data exchange
- Post-processing (visualization)



## CHRONO: Visualization and Post-Processing

- Rendering very complex scenes with more than one million components
- Rendering takes longer than simulating
- Pursuing a rendering pipeline that leverages parallel computing

# Fluid Dynamics and Fluid-Solid Interaction



# Rendering Pipeline: Problem Statement

- Render big data: efficiently and beautifully
- Have the flexibility to render anything
- Make the rendering process streamlined and simple
  - Provide rendering as a service

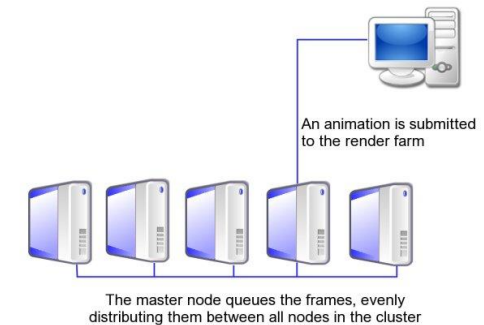
# Rendering Pipeline: From Data to Movie

- Example: Tire-Terrain Simulation
  - Data
    - Sequence of Height Maps
    - Render Settings File
  - Cluster
    - Submit data and settings to cluster remotely
    - Schedule jobs and render
  - Movie
    - Returned upon completion

DATA



CLUSTER



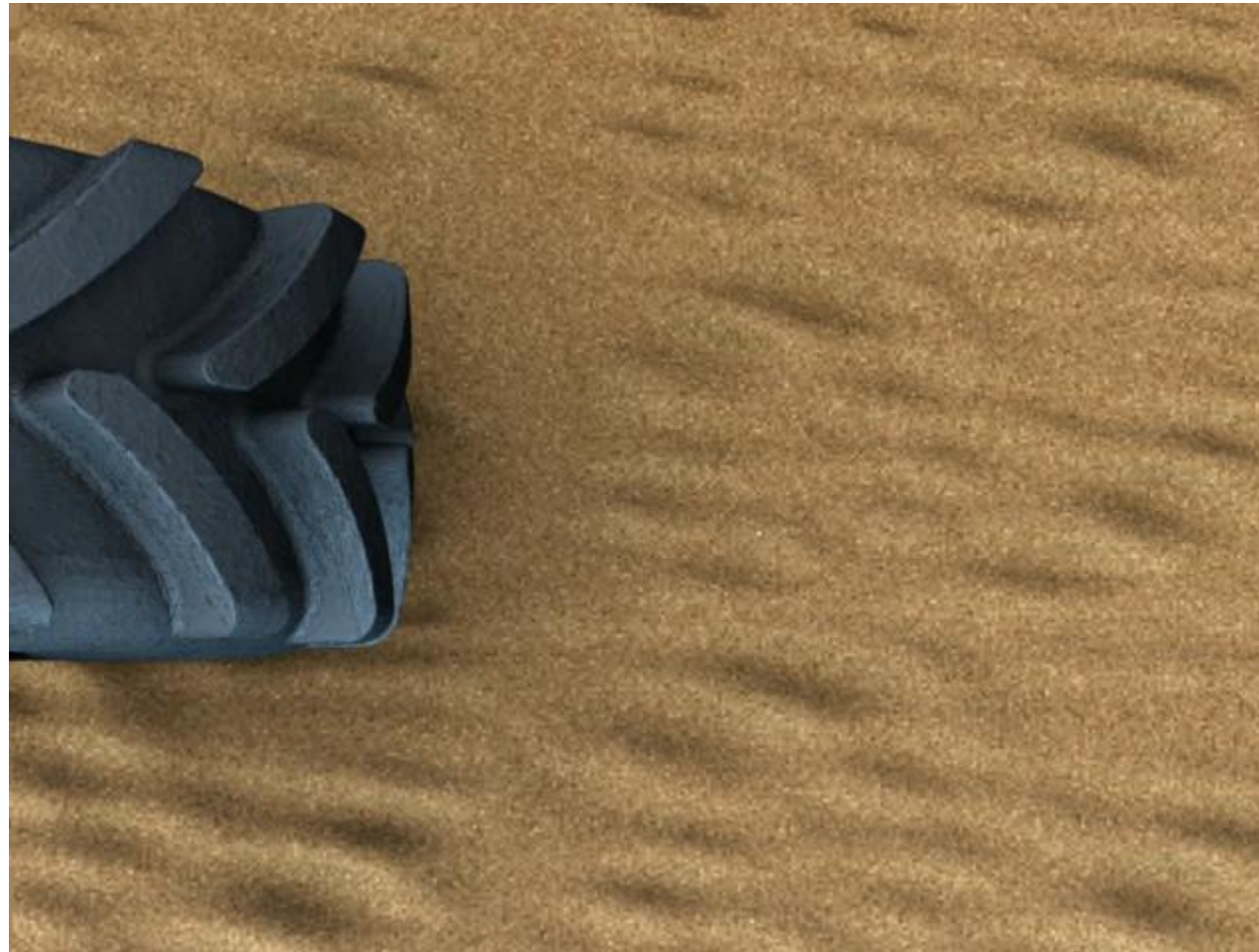
MOVIE



# Tire Rolling on Deformable Terrain



# Tire Rolling on Deformable Terrain





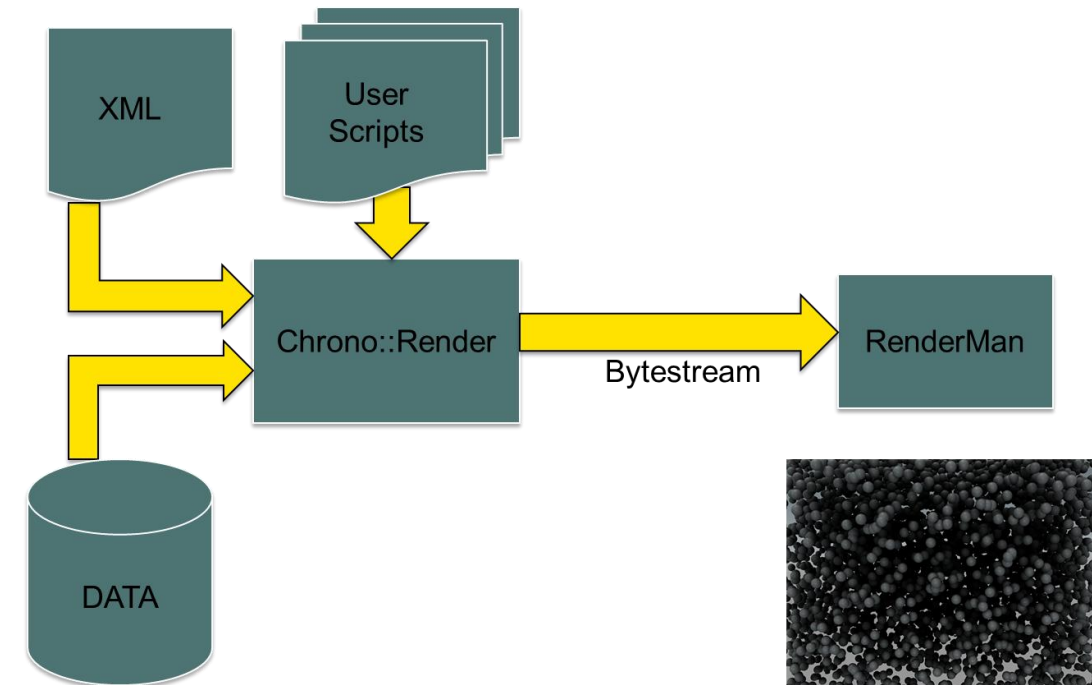
# Rendering Pipeline Uses Pixar's Renderman (PRMan)

- PRMan: Engineered to be fast, efficient, and configurable for complex scene rendering
- Pixar's PRMan: industry's rendering standard
  - Lab supercomputer can run up to 320 instances of PRMan
- Open source alternatives:
  - Aqsis
  - JrMan
  - Pixie

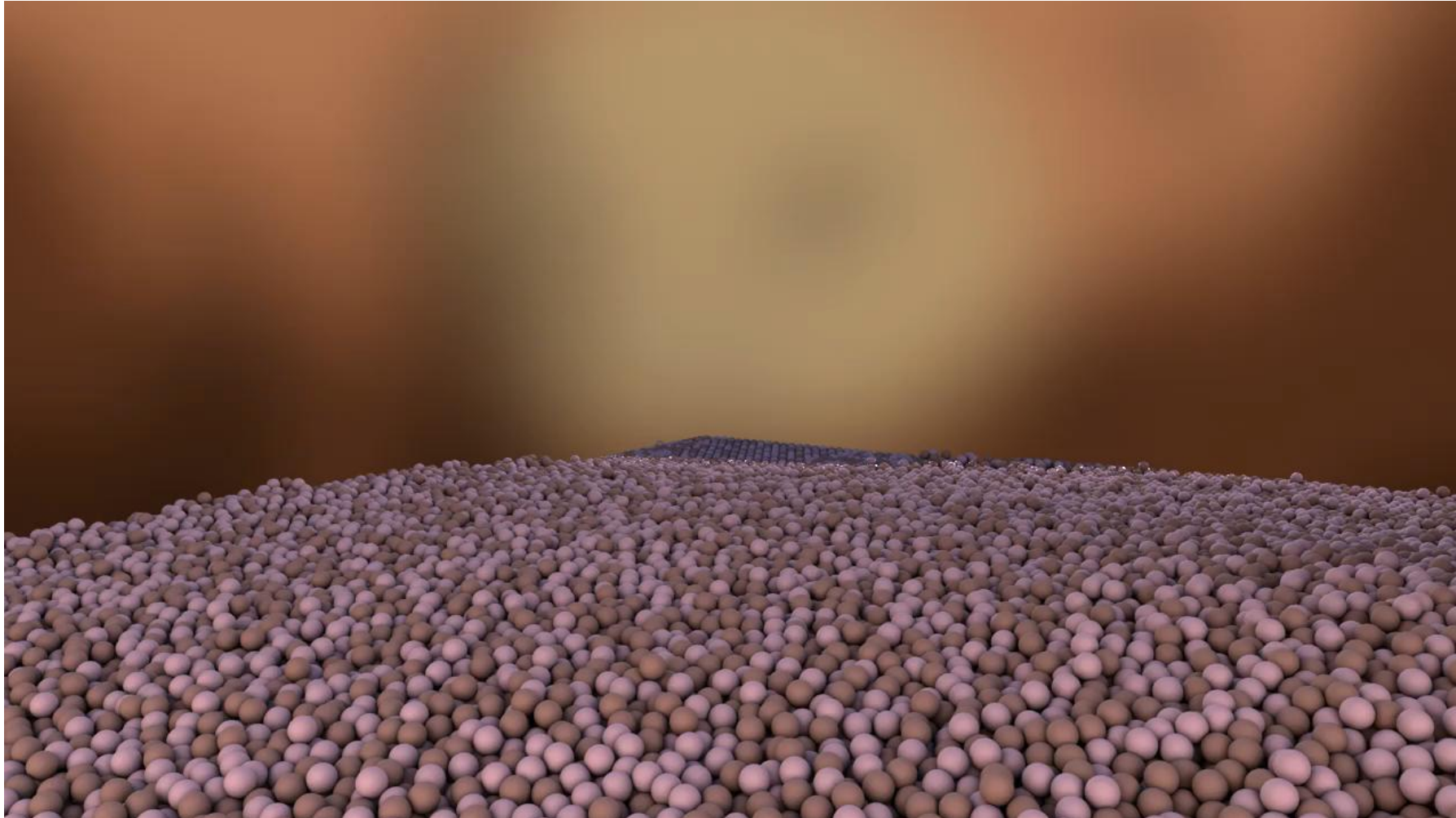
# Chrono Rendering Pipeline:



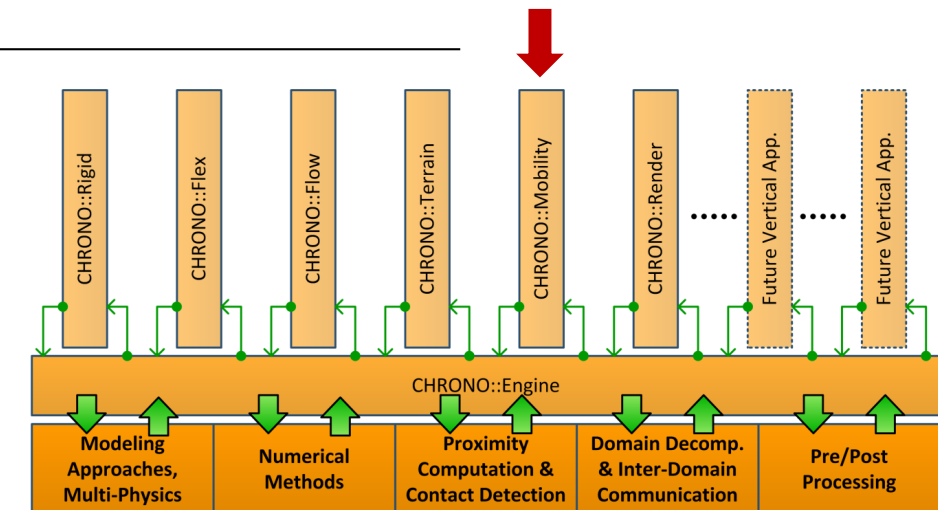
- RenderMan requires a lot of work to configure and optimize correctly
  - Not aimed at science and engineering communities
- Chrono::Render tailored to science and engineering
- Chrono::Render - What is it?
  - C++ binaries, simple Python scripting interface, and succinct XML specification



# Light Robot Operating on Discrete Terrain



# Chrono::Mobility



# Terramechanics Modeling Methodologies

1. Empirical methods
  - WES numerics, NATO Reference Mobility Model (NRMM)
2. Semi-analytical
  - Bekker-Reece vertical pressure/sinkage relation
  - Janosi-Hanamoto slip/shear relationship
  - Wong/Reece plastic equilibrium approach
3. Physics-based
  - Finite Element Analysis
  - Particle/Discrete Element methods (DEM, DVI)
  - Meshless/Lagrangian Methods (SPH, MPM, etc.)

# Terramechanics for Vehicle Mobility, Remarks

- Empirical methods have limited predictive attributes for general purpose vehicle mobility
- Semi-Analytical methods have been applied to mobility studies with some success
  - See: Trease, Holtz, Azimi, Schmid, Harnisch, Slattengren
  - Limitations due to some (but not necessarily all) of the following assumptions:
    1. Tire geometry is 2-D, circular in shape
    2. Wheel moves forward at a constant velocity and spin rate
    3. Wheel moves parallel to flat ground
    4. Soil is homogenous, perfectly plastic medium
- FEA or DEM are accurate, but computationally expensive
  - Madsen/Heyn/Negrut/Lamb (demonstrated shortly)

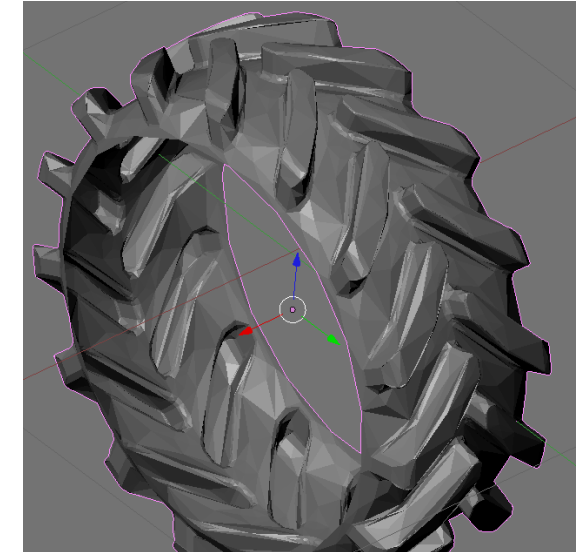
# Chrono::Mobility – Goals

- Develop general purpose simulation capability for analysis of wheeled/tracked vehicle mobility on deformable terrain
  - a) Handle 3-D tire/track geometry to accurately estimate contact patch size and shape
  - b) Handle general 3-D terrain geometry to allow for realistic mobility scenarios
  - c) Represent the terrain in a way that considers soil stress state and loading history in a volumetric sense, depending on soil type
    - Cohesive soils – compaction
    - Dry granular soils – shear failure and flow
    - Brittle soils – fracture, shear failure and flow

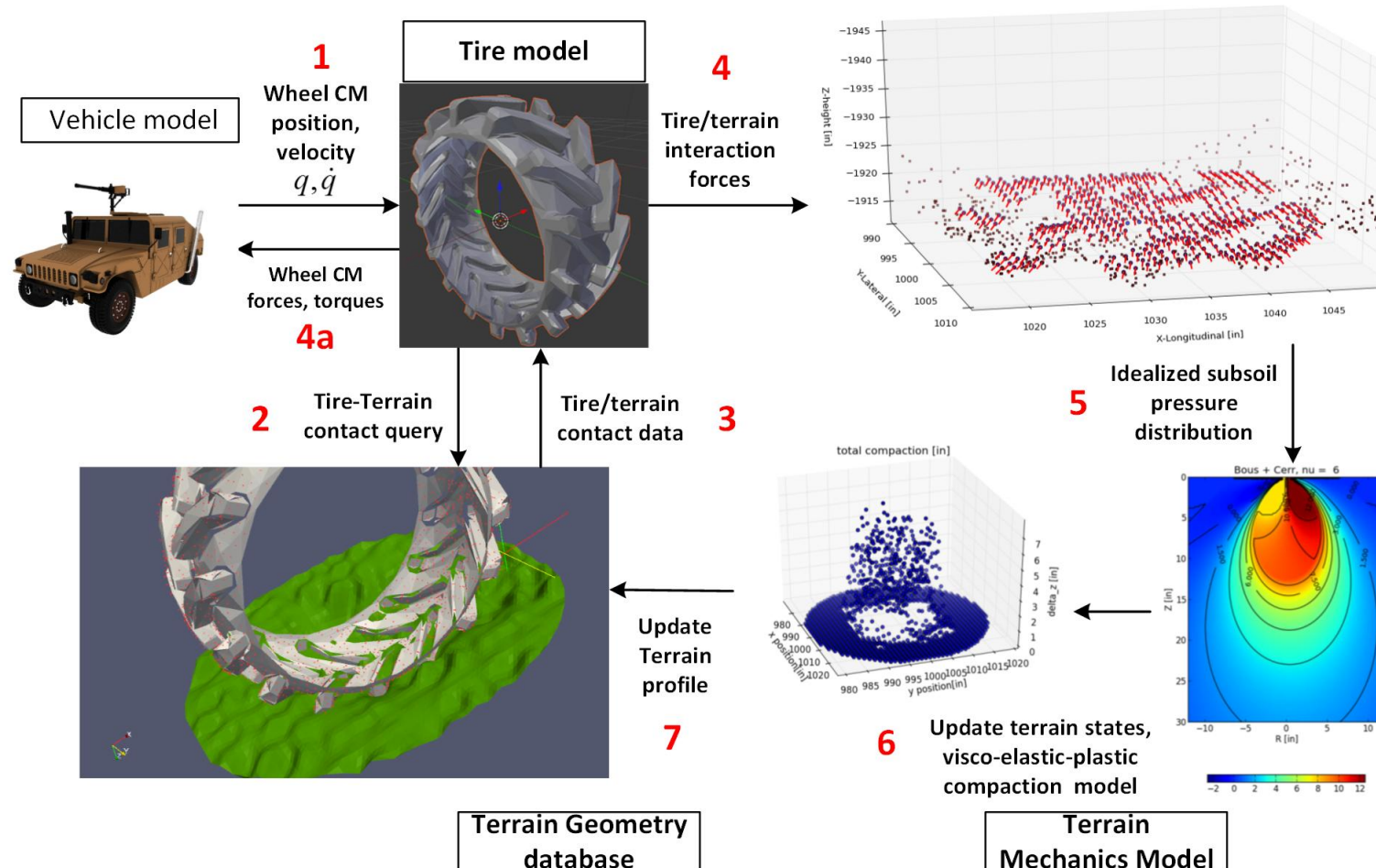


# Traction Element Geometry Representation

- 3-D geometry description for tire/terrain collision query
  - Discretized at a resolution to capture tread/lug geometry
- APIs modularized so that terrain database accepts generalized traction geometry when queried
- Directly use Wavefront (.obj) solid models (top)
  - Captures complicated tread/lug geometry
- Can also represent vehicle hull geometry



# Simulation Framework

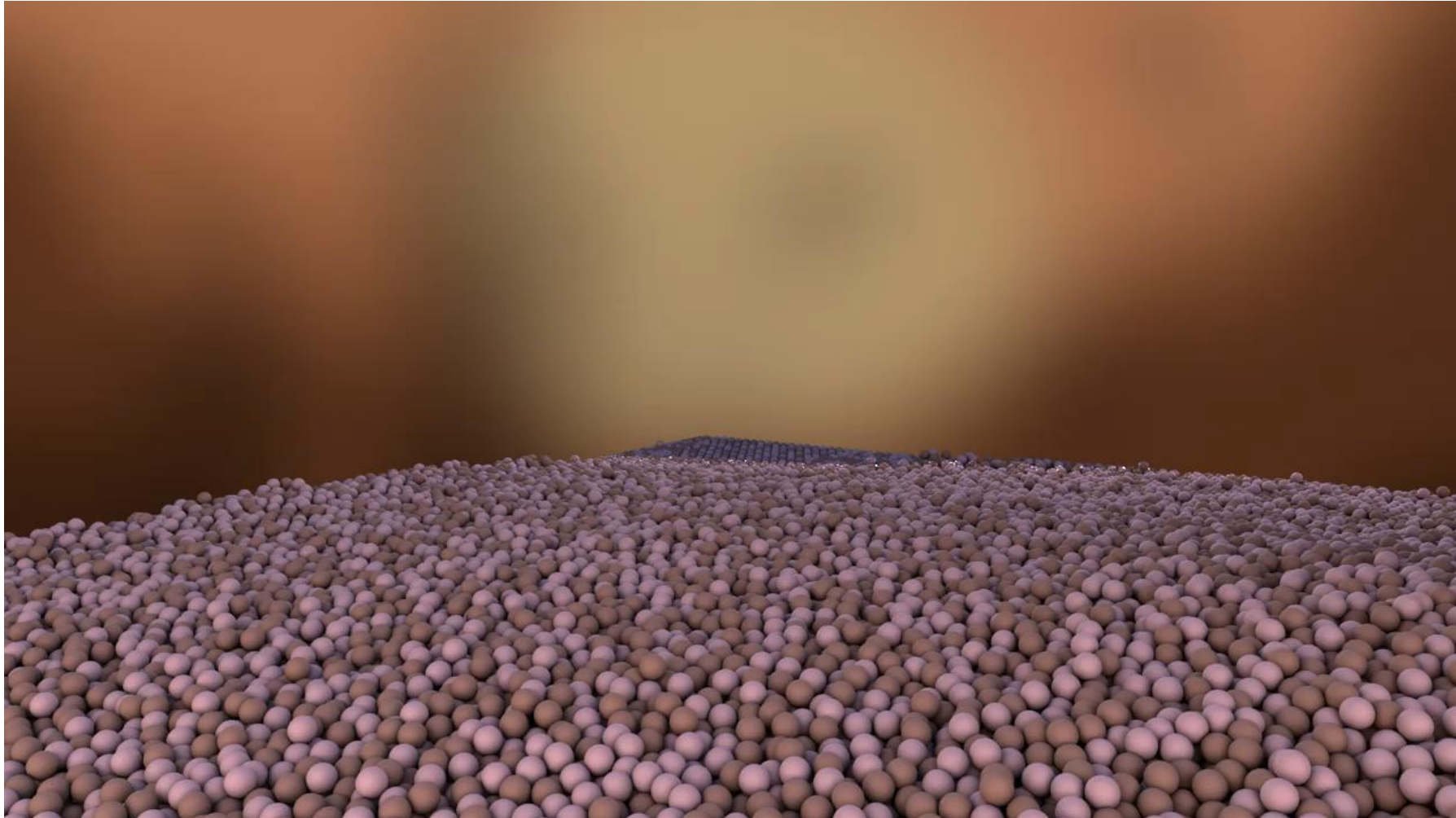




# Chrono::Mobility, Today

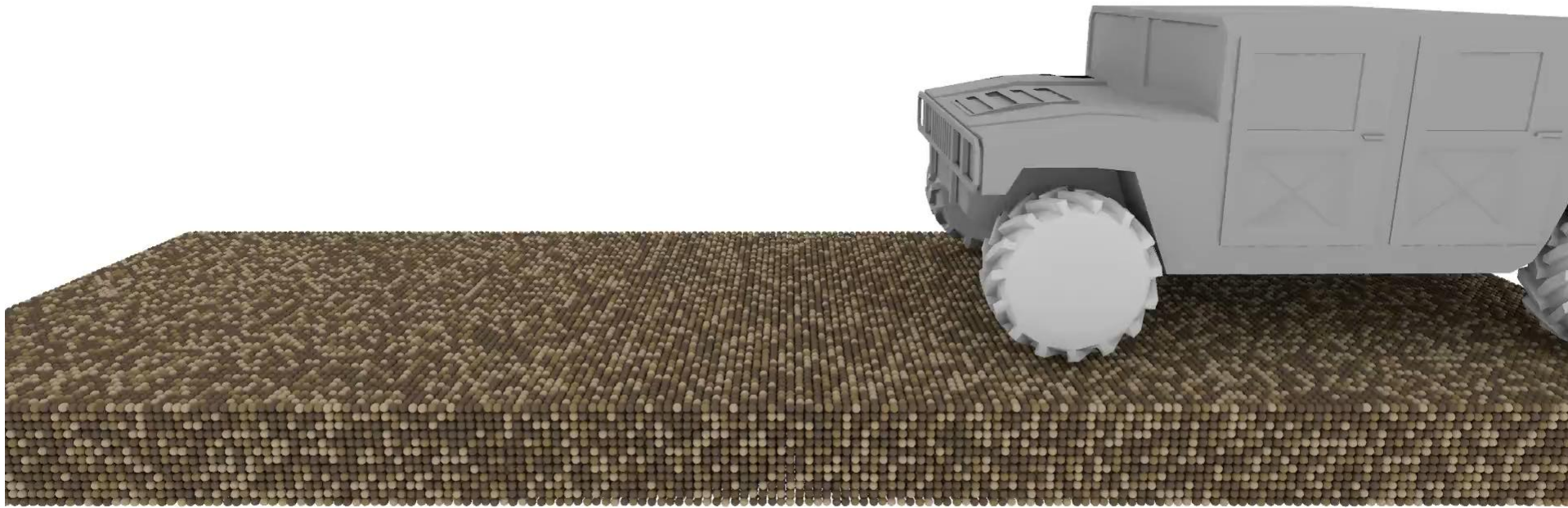
- Multibody dynamics vehicle model entirely in **Chrono**
  - Generalized 3-D tire/track and terrain geometry representations
  - Visco-elastic-plastic soil model captures soil compaction due to vehicle loads
- Leverages other members of the **Chrono** family
  - Based on Standard Tire Interface (STI) & Vehicle Terrain Interface VTI
- Discrete terrain simulation carried out in the same framework

# Light Robot Operating on Discrete Terrain

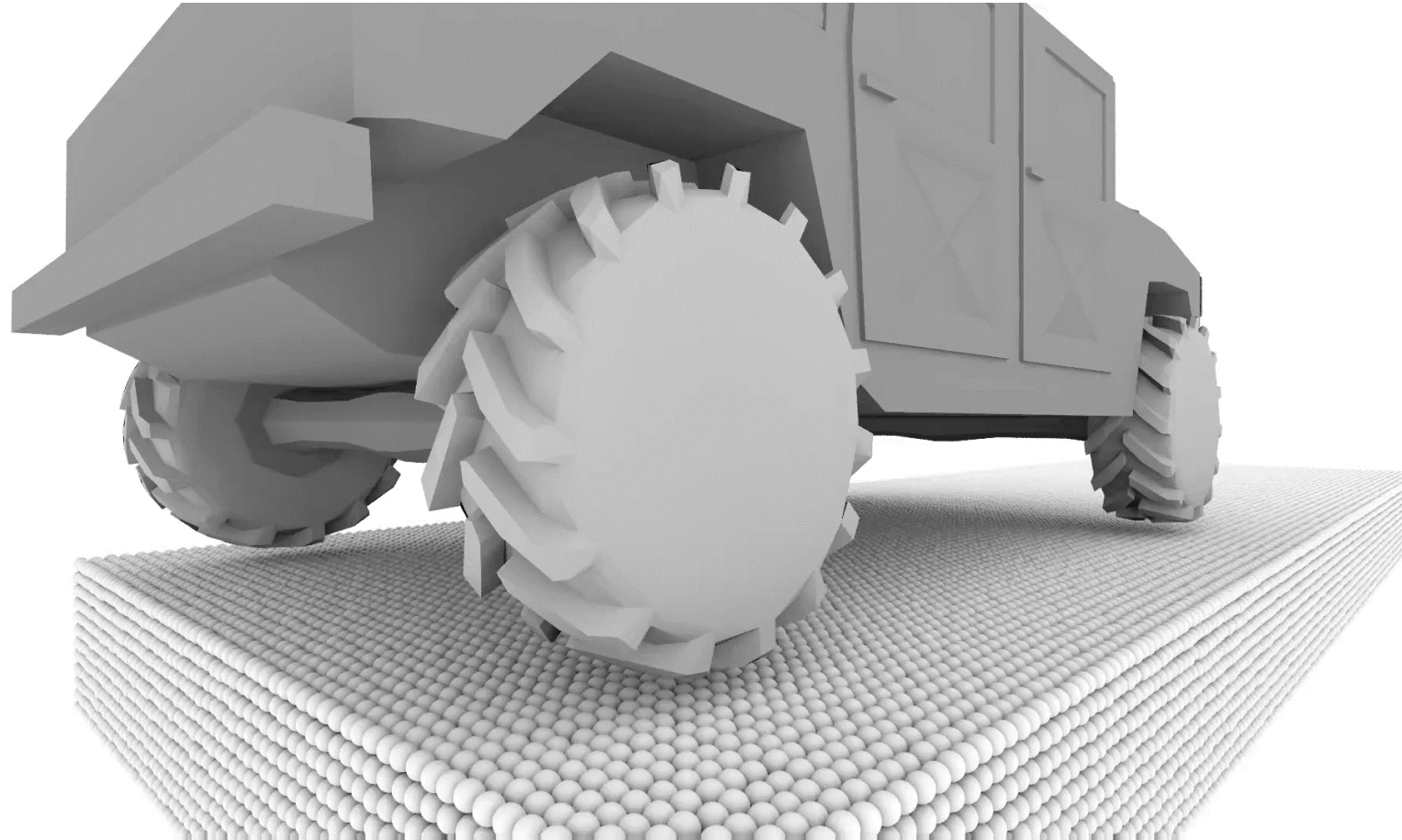




# Mobility on Granular Terrain w/ Cohesion

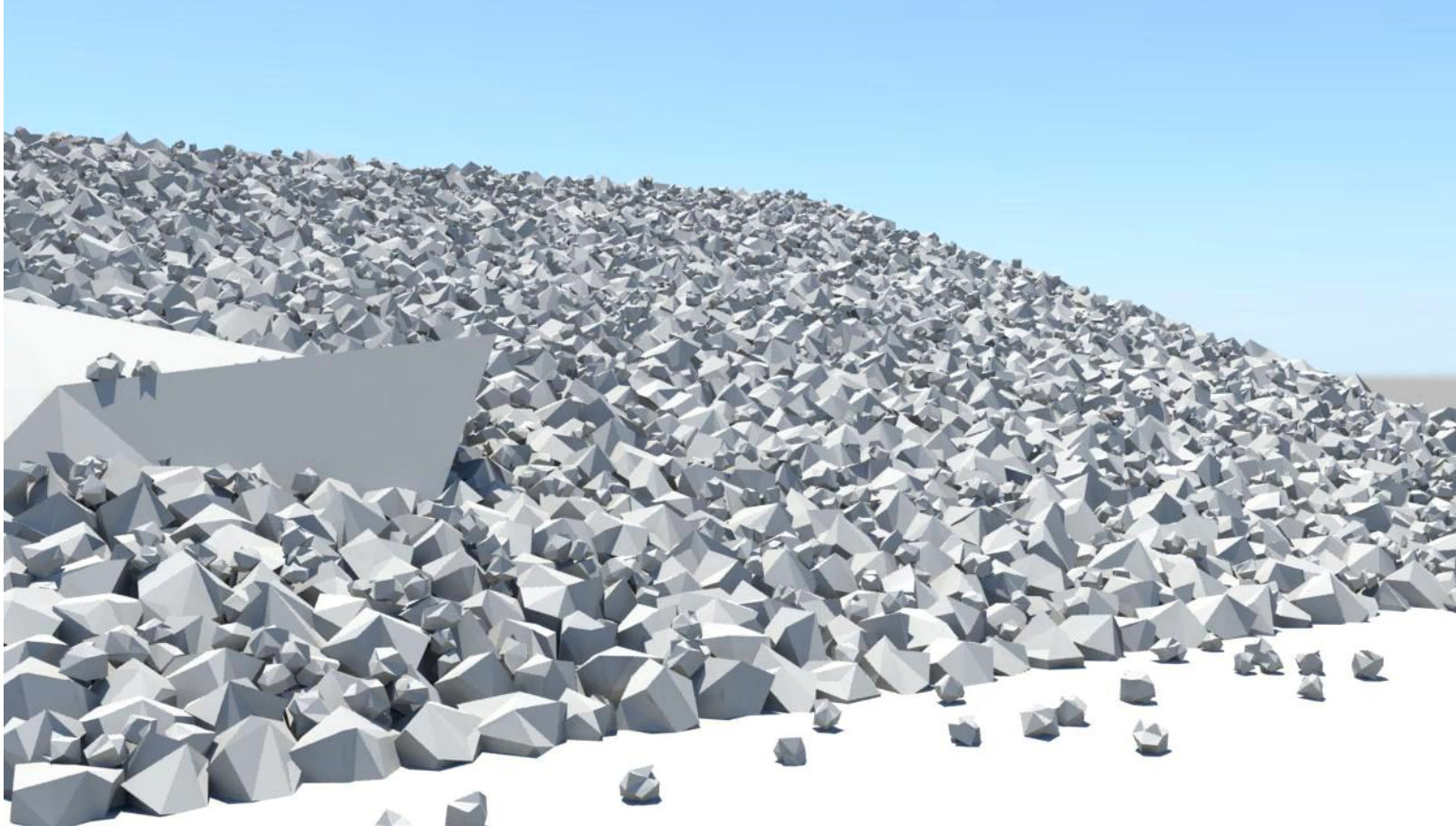


# Mobility on Granular Terrain w/ Cohesion: Close-Up



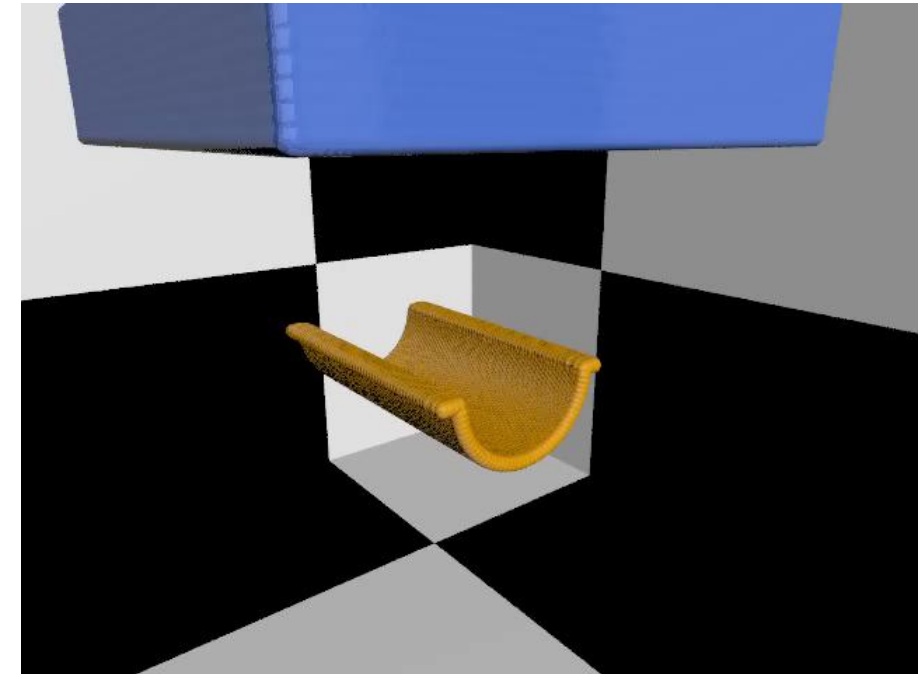
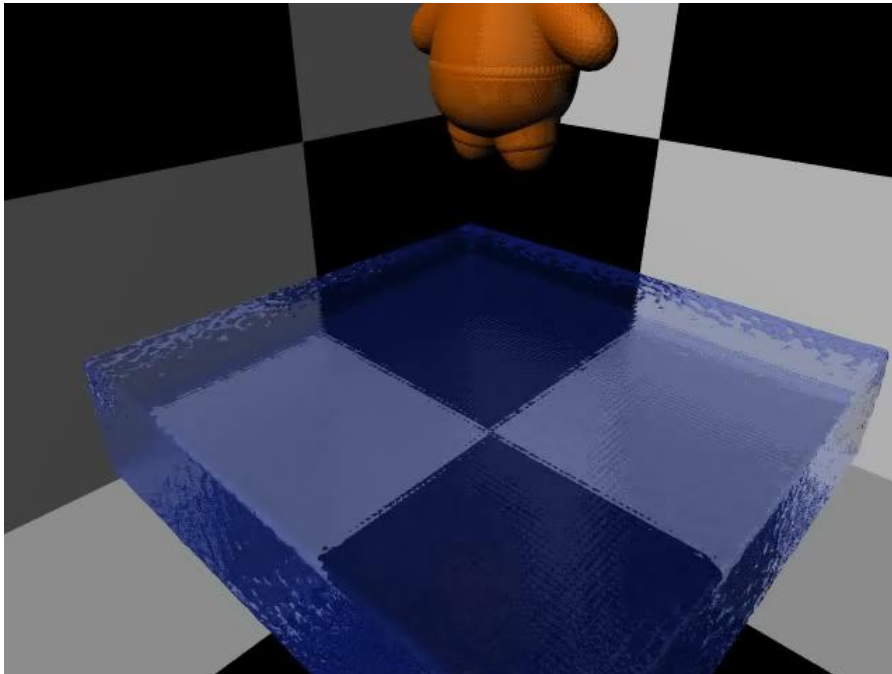


# What Can You Do With a Validated Predictive Tool?



# Fording, First Cut

# Fording, Future Plans: Coupled Fluid-Structure Interaction



9.3 years of GPU time for simulating Fluid-Solid Interaction problems

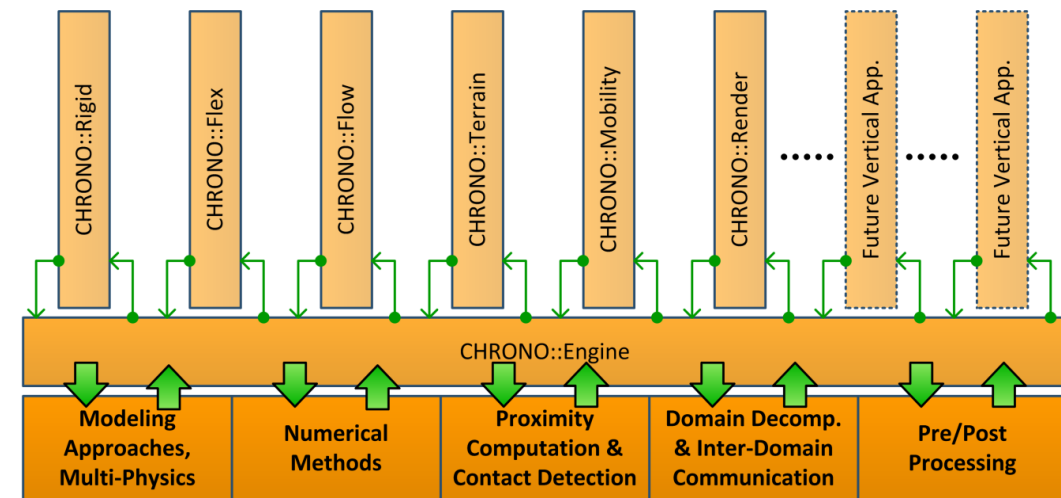
# Departing Thoughts

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# Chrono – The Long View

- **Chrono**-effort focused on four thrusts:

1. Validation – useful
2. Pre/Post – friendly
3. New features – versatile
4. Leverage advanced computing – fast

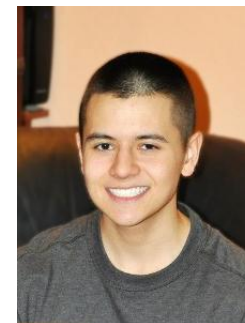
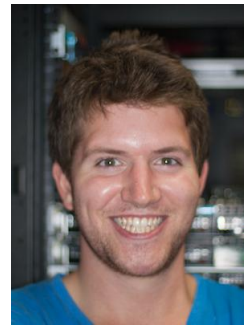


# Wisconsin Applied Computing Center

- Our group, Computational Dynamics, has 12 members
  - Three Faculty/Researchers...



- Nine Graduate and Undergraduate Students...





## Closing Remarks

- We are focused on physics-based simulation
- Vision:
  - Solve real-world problems (pursue relevant questions)
  - Put computers and good ideas to work
  - Build upon partnerships and collaborations
  - Make outcomes of our work available to users: release early, release often (BSD-3 license)
- Approaching physics-based simulation in a holistic fashion through **Chrono**
  - Modeling + numerical solution + visualization
  - Rely on emerging hardware for fast simulation

# Thank You.

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Simulation Based Engineering Lab

Wisconsin Applied Computing Center

PPT presentation & animations will be available on-line for download.